AFRL-SR-BL-TR-01-

0431

# REPORT DOCUMENTATION PAGE



| 1. AGENCY USE ONLY (Leave blank) | 2. REPORT DATE | 3. REPORT TYPE AND DATES COVERED |
|---|---|---|
| | June 19, 2001 | Final Report June 1, 1995-December 14, 2000 |

**4. TITLE AND SUBTITLE**
AFOSR/DARPA Consortium for Crystal Growth Research-Integrated Intelligent Modeling, Design and Control of Crystal Growth Processes

**5. FUNDING NUMBERS**
MURI Grant No.
F 49620-95-1-0407

**6. AUTHOR(S)**
PI: V. Prasad, Co-PI's: M. Dudley, J.E. Flaherty, M.Gevelber, J. Glimm, M. Gunzburger, F. Ladeinde, A. Maniatty, M.H.N. Naraghi, M.S. Shephard, J. Turner

**7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)**
SUNY at Stony Brook, Rensselaer Polytechnic Institute, Boston University, Arizona State University/Florida A&M University,
Iowa State University, Manhattan College

**8. PERFORMING ORGANIZATION REPORT NUMBER**

**9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)**
Marc Jacobs
AFOSR/NM
801 North Randolph Street, Rm.732
Arlington, VA 22203-1977



**11. SUPPLEMENTARY NOTES**

**12a. DISTRIBUTION / AVAILABILITY STATEMENT**
Approved for public release, distribution unlimited



**12b. DISTRIBUTION CODE**

**13. ABSTRACT** *(Maximum 200 Words)*

Growth of single crystals is the critical beginning step for electronic, opto-electronic, MEMS and many other devices. This MURI program took an integrated approach towards modeling, design and control of crystal growth processes and in conjunction with growth and characterization experiments developed much better understanding of growth phenomena and materials defects. It led to the development of most comprehensive and accurate models that account for conduction, convection and volumetric, spectral radiation heat transfer, oscillatory and turbulent flows, transport and segregation of dopants and impurities, phase change, an applied magnetic and/or electric field, and generation and multiplication of crystal defects. Using state-of-the-art adaptive grid generation techniques and parallel algorithms, the models can perform three-dimensional, dynamic simulations. While establishing white beam x-ray topography as the leading technique for crystal characterization, this research led to many new theories for grow
th behavior and defects. Advanced model-based control algorithms were developed for in-situ synthesis and Czochralski growth. Notable among many successful technology transfer projects are: AFRL-developed one-step in-situ synthesis and growth of indium phosphide crystals, growth of large diameter silicon carbide crystals, 500 mm diameter silicon tube growth, transport model for hydrothermal growth, wire saw technology and high yield polysilicon production. Besides involving numerous faculty, the project succeeded in training a large number of postdoctoral fellows and undergraduate and graduate students in crystal growth.

| 14. SUBJECT TERMS | 15. NUMBER OF PAGES |
|---|---|
| crystal growth, semiconductor materials, process modeling, crystal characterization, process control | 34 |
| | 16. PRICE CODE |

| 17. SECURITY CLASSIFICATION OF REPORT | 18. SECURITY CLASSIFICATION OF THIS PAGE | 19. SECURITY CLASSIFICATION OF ABSTRACT | 20. LIMITATION OF ABSTRACT |
|---|---|---|---|
| U | U | U | UU |

# AFOSR / DARPA
# Consortium for Crystal Growth Research

## Integrated Intelligent Modeling, Design and Control of Crystal Growth Processes

MURI Grant No. F 49620 - 95 - 1 - 0407

**1995 - 2000**

**Director: V. Prasad**
**State University of New York at Stony Brook**

**INTEGRATED INTELLIGENT MODELING, DESIGN AND CONTROL OF CRYSTAL GROWTH PROCESSES**

## List of Contents

## 1. RESEARCH OBJECTIVES

The growth of single crystals is the critical beginning step for electronic and opto-electronic device fabrication. Monolithic microcircuits are built, quite literally, upon a foundation of single-crystal materials. The distinctive properties of these materials have a powerful influence on the characteristics, capabilities, and limitations of the devices fabricated on them. They are also crucial to many other defense and commercial technologies, e.g., light-wave communications, fiber optics, photo-refraction, lasers, sensors, detectors, solar cells, and micro-electromechanical systems (MEMS). In all of these applications, the requirements of semiconductor materials include a high crystallographic perfection, very low defect density, uniform and low resistivity gradient, optimum and consistent dopant distribution, minimum and uniform impurity concentration, and high level of electrical, optical and mechanical properties. In addition, the high yield and high performance device manufacturing requires large diameter crystals. Crystal growth, therefore, has been a focal point of intense applied research in recent years and significant progress has been made in many areas. Our scientific and technological understanding of bulk crystal growth processes is much improved today. However, research on various aspects of these processes such as growth techniques, process modeling and simulation, stresses in as-grown crystals, material characterization, defects and dislocations, process control, and process design and development has been performed mostly independent of each other. The primary goal of this MURI program has been to take an integrated approach towards intelligent modeling, design and control of crystal growth processes to bring major scientific and technological advancements in this field, and help the defense and commercial research programs in crystal growth. The research objectives of this MURI program were therefore,

- to establish a multi-disciplinary, university/industry/DOD laboratory research program in crystal growth,
- to combine the separate strengths of materials science, thermo-fluid sciences, applied mechanics, control theory, computational mathematics, software engineering, design and optimization and other disciplines of engineering,
- to produce a novel capability for intelligent modeling, simulation, design and control of growth processes,
- to bring major scientific and technological advancements in this field,
- to help DOD and industrial research programs in crystal growth and related areas,
- to facilitate technology transfer for commercialization, and
- to provide multi-disciplinary training to scientists and engineers.

To achieve these goals, the Consortium took a multi-faceted approach and its major research objectives as stated in the original proposal were as follows:

- Develop comprehensive process models to account for all important physical phenomena associated with melt growth processes.
- Bring major advancements in computational techniques to model three-dimensional processes involving multiphase systems with free and moving interfaces in irregular domains.
- Contribute significantly to the high-level techniques of grid refinement, domain decomposition, and adaptive solution procedure.
- Develop parallel processing algorithms employing efficient schemes for load balancing and element migration for complex large-scale materials processing problems.

- Construct a high-resolution predictive tool (modeling and simulation code) and video animation algorithm for materials processes, particularly crystal growth.
- Make predictions of stresses and segregation of dopant and impurities key components of the model.
- Establish correlation between thermal and stress fields in as-grown crystals and its effect on defect generation and propagation.
- Develop better scientific understanding of the crystal growth processes involving large melts, high pressures, magnetic field and other physical effects.
- Use the crystal characterization methods to develop theory of materials defects and conditions that promote them.
- Design an intelligent control system to achieve optimal process conditions for better quality of crystal, including reduction/elimination of defects and twins.
- Develop correlation among the predictions, experimental data, and crystal microstructure and dislocations.
- Work closely with industry and DOD laboratory and use them as test beds to facilitate immediate transfer of technology.

On applications side, the original proposal focused primarily on:

(a) To improve scientific and technological understanding of high pressure LEC growth leading to the design and development of ultra-high pressure crystal growth processes,

(b) To examine the critical issues associated with the Cz and LEC growth of large diameter Si, GaAs and InP crystals of better quality,

(c) Apply model-based intelligent system design and control strategies to bulk crystal growth processes.

(d) Develop commercially viable techniques for "one-step" in-situ synthesis and high pressure growth of III-V compound crystals.

Since the model developed for high pressure crystal growth processes could be easily used for many other multiphase, multicomponent systems with moving interfaces as well as for the design of crystal growth systems, the research objectives of this MURI program were significantly expanded to include,

- Design, fabrication and testing of the next generation high pressure crystal growth system (an AFOSR STTR project in partnership with GT Equipment Technologies, Inc.),
- Modeling of hydrothermal crystal growth (USAF Research Lab at Hanscom and industry),
- Modeling and simulation of bulk growth of SiC crystals using physical vapor transport (a BMDO project to Sterling Semiconductor and a DARPA project to Advanced Technology Materials, Inc.),
- Modeling and system design of large diameter silicon tube growth (ASE Americas, Inc.),
- Modeling of directional solidification (Bridgman-Stockbarger growth) under the influence of thermoelectric and magnetohydrodynamics effects (NASA Microgravity Material Science Program),
- Simulation of coating of fibers using chemical vapor deposition (USAF Materials Laboratory at Wright-Paterson and Centric Engineering),
- Modeling of the CVD process for newly-proposed methods for polysilicon production (NSF SBIR project through GT Equipment Technologies, Inc.),

- Reactive flow simulation of epi-layer growth (General Semiconductor, Inc), and
- Use of X-ray topographic characterization technique to help DARPA, ARO and USAF (Research Lab at Wright Paterson) research programs in SiC growth through Cree Research and Advanced Technology Materials, Inc.

These projects and other Consortium-led initiatives have resulted in several new partnerships.

## 2. ACCOMPLISHMENTS /NEW FINDINGS

### 2.1 Physics-based Process Model

Efforts under the aegis of the Consortium has led to the development of a powerful computer model, MASTRAPP, which is capable of three-dimensional simulation of crystal growth type processes. The MASTRAPP model incorporates all the physically complex phenomena associated with these processes, the prominent ones being:

- transport of mass, momentum and energy in two and three dimensions,
- materials with varying thermophysical properties and phases,
- flow oscillations and turbulence,
- buoyancy and surface tension forces,
- crystal and crucible rotations,
- transport of dopant and impurities and segregation phenomena,
- spectral (wavelength-dependent) radiation heat transfer,
- volumetric radiation through participating media,
- applied magnetic and thermoelectric fields (Peltier, Thomson, Seebeck and Joule effects),
- phase-change phenomena,
- moving and deformable interfaces,
- thermal-elasto-viscoplastic behavior.
- dislocation mechanics in the growing crystal.

A unified approach for solid, liquid and gas phases allows direct interaction among the melt and gas flows, liquid encapsulant, solid crystal and other components of the system. We have developed comprehensive models for crystal growth processes with the following features:

**Conservation Equations.** Full implementation has been achieved in three-dimensional formulation and application of transport equations with appropriate coupling for phase-change type processes. The moving interfaces have been treated in closed conjunction with the transport equations. The resulting computer code, MASTRAPP, has emerged as the leading crystal growth simulation model and is being extensively used by the industry and academia.

**Volumetric, Spectral Radiation Heat Transfer.** A comprehensive surface and volume radiation heat transfer model for crystal growth was developed and linked to MASTRAPP[1]. The model is capable of handling many complexities introduced by radiation heat transfer in crystal growth processes, such as, spectral considerations and blockage (shadowing) effects produced by inner and/or outer obstructing bodies. This is the only existing model that analyzes such complex problem efficiently. Also, it is the first model for radiative analysis of irregular shaped axisymmetric configurations which can also be used for the analysis of radiative heat transfer in many other axisymmetric configurations, such as, rocket thrust and plug chambers.

The model was used to study the effect of radiation heat transfer for Czochralski growth of Yttrium Aluminum Garnet (YAG). An important characteristics of YAG is that the heat transfer

[1] Multizone Adaptive Scheme for Transport and Phase-change Processes

by radiation is the dominant mode of heat transfer. In this study the surrounding temperatures of the crucible (top surface and side wall of the melt) were varied. The results show that the temperature distribution within crystal, as well as, the melt-crystal interface shape are highly dependent on these temperature. An interesting application of the present model is to determine the optimum surrounding temperature history during the growth process. It should be noted that the surrounding temperatures can be easily controlled by adjusting crucible heaters. The objective of this optimization is to keep the temperature gradient low and the interface near-flat.

The radiation model was further improved to analyze axisymmetric configurations involving non-homogenous radiative properties. The results based on this new feature of the radiation model agreed well with the existing results for simplified solutions. Although the non-homogenous properties for crystals are not well known this feature of the model allows obtaining more accurate results when such properties are available.

**Turbulent Flow and Oxygen Transport in very Large Diameter Silicon Crystal Growth.** In the case of large diameter silicon growth (e.g., 200 to 300 *mm)*, the melt flow is turbulent and most of the previously developed models are not applicable. In addition, the strong swirl flow induced by the rotations of both crystal and crucible makes the standard $k$-$\varepsilon$ turbulence model inappropriate. Four different turbulence models: standard $k$-$\varepsilon$ model (SKM), low Reynolds number model (LRM), renormalized group (RNG) model, and algebraic stress model (ASM), were examined to investigate their suitability for crystal growth simulations. Application of these models to a differentially-heated cavity and a comparison with experimental data reveal that the ASM and RNG $k$-$\varepsilon$ model give the best results. The RNG turbulence-model based code is able to predict the laminar flows with same accuracy as a laminar model. It has allowed the simulation of 300 *mm* diameter silicon growth under realistic conditions. To meet the technological demand of electronics industry and grow 300 *mm* dia. crystals of very high quality, it is extremely important that we understand the role of turbulence in Si melt.

Renormalization group (RNG) k-ε model was successfully incorporated into MASTRAPP2d, and the effects of buoyancy and crystal and crucible rotations on the melt flow and heat transfer in large Cz systems were studied. These results show that the flow structure of the melt is highly dependent on the relative strength of buoyancy and system rotations. The intensity of turbulence as measured by the turbulent viscosity increases with Grashof number. Rotations of both crystal and crucible are seen to increase the turbulence intensity in general. However, when the flow state transits from buoyancy dominant to rotation dominant, the intensity of turbulence decreases with increasing rotation rate.

**Transport of Dopant or Impurities and Macrosegregation.** Chemical inhomogeneity of the crystal due to solute segregation both at macroscopic and microscopic levels, limits the quality of the crystal. The understanding and prediction of such segregation phenomena are critical to crystal growers. Macrosegregation in the crystal is primarily controlled by the transport of dopant and/or impurities in the melt. This transport process is intrinsically transient and has different time and length scales from other transport phenomena such as the transfer of momentum and heat. A special scheme has been developed to treat this multi-time scale problem, study the macrosegregation phenomena, and predict the radial and axial distributions of dopants and impurities. It is a two-time level approach in which a much larger time scale of momentum and heat transfer is treated through quasi-steady state process, but the solute transport is treated at a much smaller time level. Complex thermal and solutal transport mechanisms of dopant in a HPLEC InP growth process have been investigated in detail. The model-predicted dopant distributions at the crystal/melt interface in both longitudinal and axial directions, agree well with the experimental observations. Indeed, this is the first time that a model has succeeded in predicting the radial segregation phenomena in a dynamic system and demonstrate that the

commonly used BPS model and its modifications have severe limitations. Efforts have been made to extend this model to the growth conditions of large crystals (300 *mm* diameter Si) as well as to microsegregation of dopant, i.e., striations in crystals.

**Effects of an Applied Magnetic Field.** An applied magnetic field can successfully suppress convection in the melt and can be used to eliminate turbulent fluctuations and oscillations near the melt/crystal interface and hence the crystal quality. The model has therefore been extended to include the effects of an applied magnetic field. Extensive calculations have been performed to examine the relationship between the semiconductor melt shape and size and the direction and strength of the magnetic field. In fact, this is the first model that can show under what conditions the oscillations can be suppressed by applying a magnetic field. All previous models assume that the magnetic field is strong enough to eliminate the oscillations and then predict the melt flow. To develop basic understanding of the physical phenomena, a cavity with differentially heated side walls was also considered. The results indicate that the magnetic field is much more effective in suppressing the strength of the convective flow as well as flow oscillations when its direction crosses the direction of the primary flow in the melt. This has strong implications in the design of the MCz (Magnetic Czochralski) growth process.

**Effects of an Applied Electric Field.** Owing to its importance in many applications, the fundamental aspects of direction solidification have received much attention in recent years. Many of these studies are devoted to studying the effects of heat and mass transfer on growth rate and interface morphology. One experimental technique that has been successfully applied to study the directional solidification of single phase and multi-phase systems is Peltier Interface Demarcation (PID). PID is achieved by passing a current pulse through the directionally solidifying melt to create a thermal perturbation at the solid/liquid interface due to the Peltier effect. This results in a morphological (chemical, microstructural, and/or strain) anomaly at the solid/liquid interface at the instant of the current pulse. Due to the presence of the electric current, additional thermoelectric responses are also observed including Thomson, Seebeck and Joule effects. Different from the Peltier effect, the Joule and Thomson effects are volumetric heat production and absorption mechanisms and occur not only in the vicinity of the solid/liquid interface but throughout the bulk liquid and solid. In addition to the thermoelectric effects, a magnetohydrodynamic (MHD) effect is also observed in the presence of electron motion in the magnetic field induced by the electric field. In a gravitational environment, the MHD effect can interact with buoyancy convection so as to complicate the transport of heat and mass during directional solidification and interface demarcation. A model has been developed to account for all of these effects and have been used to simulate the Peltier effect in Bridgman growth. This research was pursued in close collaboration with Larson who is funded by NASA microgravity materials science program. This collaboration has helped in extending the model to examine the impact of thermoelectric forces on crystal growth. It seems that the thermoelectric forces can be effectively utilized to control the crystal/melt interface dynamics. This has added a new dimension to our crystal growth model.

**Thermo-Elasto-Viscoplastic Crystal Model based on Dislocation Mechanics.** A micromechanics based constitutive model was developed for InP growth, which takes into account the movement, interaction, and multiplication of dislocations in a single crystal. The model can more generally be applied to sphalerite compounds. This model assumes that viscoplastic deformation is accommodated through slip, i.e., dislocation glide, along the primary crystallographic slip systems. The dislocation density on each slip system is treated as a state variable, which is then part of the solution when solving the evolution equations for the thermally loaded crystal. The thermal and elastic components of the deformation are modeled as an expansion/contraction of the lattice and elastic stretching of the lattice, respectively. The model

has only two adjustable parameters, while the remaining parameters are measurable, physical parameters. The model was found to be capable of predicting, with reasonable accuracy, a wide range of experimental results reported in the literature. This model has been implemented into a finite element code, which is then integrated with MASTRAPP.

## 2.2 Numerical Implementation

Modeling realistic Cz, LEC and MLEK crystal growth processes offer several computational challenges. Viscous flow systems must be solved on complex two- and three-dimensional systems. The positions of the crystal/melt interface and melt/gas meniscus are unknown non-planar, time-dependent functions. The crystal/melt interface coincides with the freezing point isotherm in the system, and the melt meniscus results from a force balance between the surface tension, pressure forces, and viscous stresses. Furthermore, the fluid and temperature fields, which determine the shape and location of the interface and meniscus often exhibit oscillations. Elastic and plastic crystal deformations arise due to thermal and velocity gradients and coupled thermal, solid, and fluid fields. Mathematical models must be developed and tested; thus, a computational system should have flexibility for easy variation of differential equations and their associated initial and boundary data. Large scale multi-dimensional computation is necessary and effective parallel solution procedures are essential to achieving acceptable performance. Two adaptive numerical schemes have been developed to deal with such complex numerical problems:

- Three-dimensional multizone adaptive finite volume scheme (MASTRAPP)
- Adaptive finite element scheme with hpr-refinement

### 2.2.1 Multizone Adaptive Finite Volume Scheme (MASTRAPP)

In MASTRAPP, the governing equations are discretized and solved using the versatile finite volume technique in a non-orthogonal curvilinear coordinate system. A non-staggered grid system is used since it is better for the imposition of interfacial boundary conditions in a multiphase system. This, however, requires a higher-order interpolation to calculate the fluxes and handle the velocity-pressure coupling. The solution algorithm is similar to SIMPLER, which consists of solving a pressure equation to obtain the pressure field and a pressure-correction equation to correct the predicted velocities. However, the scheme is much more complicated since the velocity directions continually change along the coordinate lines. For the case of materials processes, it has been linked with an adaptive grid generation scheme; Multizone Adaptive Grid Generator (MAGG). This scheme is versatile in the sense that it tracks the moving interfaces accurately and at the same time maintains proper grid characteristics for accuracy. The code has been used to solve a variety of problems and is well tested for its strength and applicability. MASTRAPP is the only computer model in the world as of today that can systematically simulate the high pressure liquid-encapsulated Cz growth process for InP and other compound materials and predict the stress and segregation phenomena.

**Parallel Version of MASTRAPP.** We have also developed a two-dimensional parallel code to allow simulation of High Pressure Liquid Encapsulated Czochralski (HPLEC) crystal growth processes. HPLEC processes are more complex than low pressure processes as there are more physical phases in high pressure systems with significant effect on thermal transport in the furnace. Secondly, the re-circulatory gas flow is turbulent in nature, and requires a turbulence model for its treatment. Furthermore, the interaction between the gas and melt flows may affect the interface and meniscus conditions and growth dynamics. The strong coupling between gas flow and heat transfer requires a large number of iterations for the solutions to achieve convergence within each time step. We have modified the parallel grid generation algorithm so that the additional physical domains, *i.e.*, the gas and the encapsulant, are incorporated into the system. We have also extended the solution procedure to solve the compressible flow equations in the gas region.

### 2.2.2 Three-Dimensional FEM Code Development

The goals for this part of the research were:

- Develop systems integration tools to enable the various software components to interact, and thus, address the simulation of the entire crystal growth manufacturing process.
- Develop software tools for parallel adaptive computation that may be used to solve finite element and finite volume problems.
- Develop unstructured-grid flow analysis software that may be used to address problems in complex geometrical configurations.

Our accomplishments on these goals are as follows:

**Systems Integration.** Software to interface the three-dimensional FEM software with the two-dimensional (MASTRAPP) FVM and the discrete exhange factor radiation software was completed early in the project. This software assumed the creation of MASTRAPP3d and is capable of being integrated with it. The integration software is capable of taking input from the heating source and using it to solve complete problems with iterative coupling between the radiation and discretization technologies.

**Automatic Domain Discretization Technologies.** A key capability in automated adaptive simulations is the construction and control the meshes. SCOREC automatic domain discretization procedures developed for this purpose have been collected into a mesh generation toolkit referred to as the Meshing Environment for Geometry-based Analysis (MEGA). MEGA supports the fully automatic generation of controlled discretizations starting from domain definitions including toleranced non-manifold geometric models and discretized representations. Mega supports a wide variety of mesh generation and modification procedures including (i) isotropic meshing , (ii) boundary layer mesh generation for viscous flow calculations, (iii) curved mesh entities for higher-order methods, (iv) multiple elements through the thickness in thin model sections, (v) mesh control functions including curvature, (vi) controlled meshes in the presence of small model features, (vii) refinement and coarsening meeting specific criteria and for adaptive analysis, and (viii) octree based domain discretizations used with advanced equation discretization methods such as partition of unity and discontinuous Galerkin methods.

The toolkit nature of MEGA allows it to be easily extended to meet new requirements and to mesh models from new sources. MEGA capabilities that support this include: structures to define the geometric and mesh models and their interactions, a generalized mechanism to interact with the geometric representations, and algorithms that deal with complexities that arise in the generation of meshes for complex curved domain geometries. Mega was used to create the finite element meshes, including boundary layers, for the finite element simulation presented below.

**Object oriented adaptive analysis framework.** To facilitate the development of new adaptive analysis capabilities, a geometry-based, object oriented computational framework has been designed and implemented. This system, referred to as Trellis, is based on: (i) geometry-based structures which can support direct linkage with CAD information, (ii) careful decomposition of the geometry, physics, mathematical model, discretization and numerical methods into interacting classes, (iii) adaptive control of each step of the simulation process, and (iv) parallel solution of adaptively evolving problems.

Trellis is able to effectively support general combinations of advanced domain and equation discretization techniques. Example formulations that have been implemented include mixed finite element formulations of the biphasic equations to solve soft tissue problems, stabilized finite element formulations for non-linear solid mechanics, solid mechanics with partition of unity methods, and high order discontinuous Galerkin methods for fluid flow problems.

The Trellis simulation framework contains complete capabilities to solve problems on higher-order meshes. To support the adaptive solution on such meshes when continuous finite element fields are used variable p-order elements are supported through the careful decomposition of the shape functions into order dependent functions over entities times a blend over the element. In the case of discontinuous Galerkin methods alternative hierarchic p-version functions with selected orthogonality requirements are supported. Procedures to properly represent curved element geometries based on blending of exact mappings over entities were developed as well as alternative procedures to integrate high order simplex shaped elements.

**Parallel Data Management.** The *Rensselaer Partition Model* (RPM) provides distributed mesh data structures and information about the parallel computational environment in which a program is executing. It has a hierarchical structure with both a process and machine model that represent the actual computational nodes and their communication and memory properties. This makes it possiblethat to tailor task scheduling to a particular, possibly heterogeneous, architecture. Its structure is rich enough to handle *h*-, *p*-, and *r*-refinement and several discretization technologies including finite difference, finite volume, finite element, and partition of unity methods. Entity weightings have been used to successfully partition adaptive time marching algorithms and to create a predictive load balancing procedure where the weights were based on refinement level and the mesh rebalanced before the refinement was performed.

**Dynamic Load Balancing.** Load balancing procedures frequently use the number of elements as a measure of imbalance. However, heterogeneous costs are necessary when (*i*) using adaptive *p*-refinement, (*ii*) using spatially-dependent time steps (local refinement), (*iii*) enforcing boundary conditions, (*iv*) solving multiscale problems, (*v*) solving multiphysics problems, and (*vi*) using predictive load balancing. We have developed an element weighting scheme that can be used to address each of these needs. Such a weighting scheme was used in the simulation of a tilted three-dimensional reactor used in chemical vapor deposition of gallium-arsenide (GaAs). The problem was solved using the *MPSalsa* code developed at Sandia National Laboratories. Since computations near reacting surfaces require a greater effort than those elsewhere in the flow, a balancing procedure that was based on element interaction would be grossly inefficient. A weighted balancing on a problem with 5.5 million unknowns resulted in a 46 percent reduction in surface chemistry time and a 23 percent reduction in solution time relative to one that ignored the extra difficulty induced by reaction.

Weighting can also be used to predict and correct for imbalance prior to enrichment. Error indicator and refinement threshold values are used to assign weights to elements in proportion to the number of elements that will be created during refinement. Balancing these weights across the processors before refinement distributes the work of the enrichment process while reducing the likelihood of memory overflow during refinement. Further, for analysis techniques which require the same work per element to generate a solution, the workload in the subsequent computation is also balanced, eliminating the need for *a posteriori* load balancing.

We have developed several dynamic load balancing procedures that utilize an octree representation of the special region and mesh. These produce efficient and effective balancing procedures. They operate in parallel and the tree structure may be distributed across the processors of the parallel computer. They have a natural hierarchy and may be used for multilevel balancing strategies. They may be updated between invocations; hence, they are suitable for use with adaptive methods. Several tree traversal procedures (*e.g.,* Morton, Hilbert, and Greycode orderings) are possible. These procedures and the predictive load balancing strategies have been incorporated into the Zoltan Library of Sandia National Laboratories. This library is available for public use within the United States.

**Parallel Solution Procedures.** We have investigated adaptive multilevel (AMLI) preconditioning techniques for the iterative solution of large, sparse, linear systems. We have generated and tested a parallel, polynomial-level) preconditioner and have demonstrated its utility with quasi-minimal residual (QMR) and generalized minimum residual (GMRes) iterations. We demonstrate that the methods perform and scale well using several symmetric and asymmetric linear systems.

Efficient implementation of the solution strategy with spatially refined regions requires a method to perform an efficient, parallel, spatial coarsening. We do this using the octree structure mentioned in the previous section as follows: (*i*) an association between existing mesh vertices and nearby fine level octree vertices is determined, (*ii*) linear interpolation is used to generate prolongation (and restriction) operators relating the mesh and octree vertices, (*iii*) a coarser level is generated by the application of these transfer functions to the existing fine level, and (*iv*) steps (*ii*) and (*iii*) are repeated with successively coarser octree levels until a sufficiently coarse problem is obtained. This algorithm has been tested on three-dimensional elliptic problems With excellent performance and scalability.

We have implemented these algorithms using generic programming techniques and C++ templates. This gives us the ability to freely switch among various parallel and serial implementations provided each such implementation meets some minimum criteria for matrix and vector classes. As part of this process, we have completely divorced the matrix and vector data structures from the parallel communications requirements by the introduction of parallel classes templated on serial classes and on communications classes.

### 2.2.3 Thermo-Elasto-Viscoplastic Model Finite Element Implementation

The thermo-elasto-viscoplastic crystal constitutive model discussed above (Section 2.1) has been implemented into a three-dimensional finite element code, which has been integrated with MASTRAPP. Specifically, MASTRAPP provides the crystal geometry and temperature field as a function of time throughout the growth process. The MASTRAPP geometry information is used to generate a geometric model, and then a finite element mesh is created based on the geometric model. The temperature data is interpolated onto the finite element mesh. A radial return algorithm was developed for integrating the constitutive equations and a consistent tangent matrix formulations was derived and implemented for solving the nonlinear system equations resulting from the finite element discretization of the thermal-mechanical system. A Lagrangian mesh updating algorithm is used to simulate the growth of the crystal and also to track and update the material state. In this method, material particles are tracked to determine the evolution of their state during the growth process. The algorithm allows for the changes in the mesh due to the addition of new material.

The growth of an LEK grown InP crystal was modeled to a total length of approximately 30 mm. The crystal has a diameter of 50 mm and is grown with the <100> axis parallel to the growth direction. An initial dislocation density of $1 \times 10^{5}$ m/m$^3$ is assumed on each slip system at the solid/liquid interface. The initial axial locations were at the bottom of the initial crystal used to start the simulation, which was 8mm in length. This corresponds to the region with high dislocation density. We found a large initial growth rate on the outside diameter of the crystal where the temperature gradient is the largest. This growth rate decreases after the surface moves approximately half of a diameter from the interface surface. In addition, the difference in dislocation density may be attributed to the anisotropy in the material.

## 2.3 Characterization of InP

Characterization of structural and composition perfection of the crystal are critical to the understanding of the relation between crystal growth and defect generation. Among the techniques traditionally used to carry out such studies are etch pit analysis and transmission micorscopy (TEM). Both of these techniques suffer from innate limitations. Etch pit analysis is

destructive, changing the surface morphology of the wafer under investigation. It can only reveal defects (dislocations, precipitates and twins) intersecting the surfaces of the wafers, but can not provide information about overall defect configurations that are very crucial to crystal growers. TEM is also destructive and defects unrelated to the growth process can be introduced during the sample preparation process. In addition, the very small field view of TEM, typically in the range of a few microns, impedes its use in the study of overall growth defect microstructures in bulk crystals.

On the other hand, X-ray diffraction topography, a non-destructive and highly strain-sensitive diffraction imaging technique, is well suited to the study of the relatively low defect densities in semiconductor crystals. Synchrotron White Beam X-ray Topography (SWBXT), combined with chemical etching and Nomarski optical microscopy, has been employed to carry out studies of MLEK grown, Fe-doped [001] InP single crystals, MLEC grown, sulfur doped, [001] InP single crystals (by Bliss at USAF Research Lab. at Hanscom), as well as the GaAs wafers obtained from M/A-COM Corporation and Litton Airtron. In the case of InP, significant new insights into the following phenomena have been obtained: (1) the evolution of the interface shape during growth of S-doped InP, as revealed by growth striations, (2) plastic deformation, in both Fe- and S-doped InP, generated by thermally induced stresses during growth, and (3) the formation of growth twins in S-doped InP.

**Evolution of Interface Shape.** The growth interface in S-doped InP is rendered visible in SWBXT via strain contrast associated with growth striations. Detailed analysis of the origins of this contrast has been carried out through its investigation under various diffraction conditions. This analysis has revealed that the contrast arises through the interaction of the propagating X-ray wavefields in the crystal with lattice rotation experienced by the atomic planes close to the crystal surface. This lattice rotation is a consequence of the requirement for static equilibrium, i.e., it is produced as a result of image stresses which must exist to annul the non-zero stresses at the surface created by the variation in dopant concentration in the striated regions. The striation contrast reveals the evolution of interface shape as the crystal grows. Initially, as the crystal diameter is increased (before pulling is initiated), an interface shape which is convex to the melt was observed. Interface "turnover" was observed to occur at the point at which the crystal shoulder emerges from the melt (after initiation of pulling). Eventually, as the crystal grows, a convex interface shape is regained. Observations of this evolution qualitatively support the results of growth models (MASTRAPP).

**Plastic Deformation.** In order to investigate the distribution and type of slip dislocations observed in InP crystals, X-ray topography was carried out on a series of (001) wafers cut from the same Fe-doped boule, and on a series of (110) wafers cut from the same S-doped boule. Results were compared to the predictions of thermally-induced, excess-stress map calculations. These calculations were carried out using the thermal fields generated by MASTRAPP. For the case of the (001) wafers, the calculations predict that the excess shear stress is highest along the [010] and [100] directions, and lowest along the $[\bar{1}\,\bar{1}\,0]$ and $[1\,\bar{1}\,0]$ directions. This agrees with the dislocation density distribution in (001), Fe-doped wafers. For the case of the (110) wafers, the calculations predict that the greatest stresses are experienced at the points where the crystal emerges from the encapsulant. SWBXT observations of (110) wafers, cut parallel to the [001] growth axis of a S-doped InP boule, reveal slip bands which propagate from the outer cylindrical surface of the boule to its interior, qualitatively supporting the stress model. Significant plastic deformation is also observed to occur in the shoulder region of the boule as well as in the tail end of the boule (corresponding to the end of growth). Modeling of the thermal fields in these regions is currently being carried out using FEM model coupled with MASTRAPP.

Growth Twinning. For the case of growth-twinning, observations in [001] grown, S-doped InP were compared in detail to the famous model of Hurle regarding the formation of growth twins in

zincblende structure crystals. These observations have enabled significant new insights to be gained into this phenomenon and necessitated modifications to the original Hurle model. The significance of the present results is fivefold: (1) this is a direct observation of the nucleation of a twin on a {111} edge facet, giving rise to the replacement of a {115} external shoulder facet by a {111} one, confirming the basic principle of the Hurle model, (2) the most dangerous "grow-out" angle for [001] growth of InP from the point of view of initiating twinning is modified from 35° to 74.2°, (3) the range of $\nu$ angles for which edge facet pinning should occur in InP has been modified to $31° < \nu < 112°$, (4) for twinning to be geometrically possible in [001] crystals of zincblende structure, the range of angles for which edge facet pinning is thermodynamically favored should encompass 70.5° and/or 109.5°, and (5) the grow out angle of 35° for [001] growth, at which {111} shoulder facet formation is favored, was defined as being dangerous from the point of view of the initiation of patch twins on those external facets by a similar mechanism. Further analysis appears to indicate that InP exhibits a preference for $\{111\}_P$ edge facet formation over $\{111\}_{In}$, and a subsequent disposition to twin on $\{111\}_P$ planes rather than $\{111\}_{In}$ planes. This appears to be in accord with previous observations reported in the literature for [111] and [001] axis growth of InP, and other III-V crystals (particularly indium-containing ones). In addition, twinning was also observed to occur by a similar mechanism but which gave rise to the replacement of a {114} external shoulder facet by a {110} one. These results have serious implications on desirable growth conditions of the compound crystals and provide valuable information for the design, development and control of HPLEC processes using a process model.

### 2.4 Optimal Control of MCZ Process

Mathematical formulation and computational model has been developed to determine optimal control and design strategies for the suppression of turbulent motions in the melt and the minimization of temperature gradients in the crystal in Czochralski crystal growth processes. The methodologies developed can be used to test control mechanisms, design parameters, and optimization objectives to determine their effectiveness in improving the processes. They can also be used to effect such improvements by systematically determining optimal values of the design parameters. The controls or design parameters considered include applied magnetic fields, temperature gradients along the side wall of the crucible, and crucible and crystal rotation rates. The results show that applied magnetic fields can be very effective in reducing velocity perturbations in the melt, while side wall temperature gradients are less effective and crucible and crystal rotation rates are ineffective. The results also show that applied magnetic fields, crucible and crystal rotation rates, and side-wall temperature variations are ineffective in reducing temperature gradients in the crystal or in the melt.

Carrying out these steps involved the integration between the modeling, simulation, and control groups involved in the project. For example, the codes developed that determine optimal control and design strategies were built upon the MASTRAPP simulation codes developed by the modeling and simulation groups. The end result of our efforts is that we have developed a methodology and a suite of codes that can be used for the optimal design of Czochralski crystal growth processes. Along the way we have made many algorithmic and theoretical advances that can be used in a many other setting as well, especially those that involve the control of flows. Thus although the specific product of this part of the project is a tool that can be used by the designers of crystal growth processes, our results have and will continue to have impact on a much wider range of applications.

### 2.5 Control of In-situ Synthesis of InP

There are significant reproducibility problems with the in-situ synthesis of the InP melt for the process developed by USAF Research Laboratory at Hanscom since during the synthesis stage phosphorus vapor escapes from the melt and back-wash of InP melt that can clog the injection tube. The reasons for these problems together with what system and control structure designs can

improve yield have been investigated. The strategy is to understand key aspects of the process including the nonlinear behavior observed in the thermal dynamics of the system, the uncertainties associated with the phase transformation of phosphorus, and high position sensitivity of the process. A model has been developed to provide the insight needed to develop an appropriate system which includes characterizing the dominant dynamics, nonlinearities, disturbances, and the relation of the input, output, and measurement variables.

The model includes the important process physics including the heat transfer by convection and radiation, the phosphorus phase transformations, the bulk fluid dynamics of $N_2$ and $P_4$ gases, the momentum and mass transport of the bubbles injected into the melt, and the reaction kinetics and heat of the P and In to form InP. Sublimation is the dominant phase transformation in the process and occurs in two regimes: a) during the initial temperature ramp up and b) at saturated conditions when the phosphorus partial pressure reaches the system bulk operating pressure. Simulation of the conditions for USAF Research Lab. experimental runs reveal that the initial sublimation accounts for only 10% of the phosphorus injection, while most of the sublimation occurs at the saturated conditions. The control implication is that it is not important to control the temperature of the injector or its time rate of change. Instead, one should control the injector heat flux. In the current system configuration, that is difficult to achieve, although the new design does have controllable actuators.

The mass transport from the P-bubbles into the melt is a rate limiting step, and the total mass flux is limited by the translation time of the bubble from the injector tip to the melt-encapsulant surface. Scaling analysis of the bubble mass transport compared to the bubble velocity reveals how these competing rate limitations scale with bubble diameter. Better control of phosphorus injection would limit the amount of phosphorus that passes into the puller, which creates smoke that prevents the operator from observing the process. In terms of implementing control, measurement of the melt weight could be used for the feedback signal to control the injection process. A cascaded control structure has been proposed that compensates for variations in the thermal dynamics that occur as the phase transformation process continues.

**Advanced Control Requirements.** We have focused on two areas for improving processing capabilities: a) increasing the ability to manufacture material with new materials properties that enable new applications and/or extend the capabilities for existing applications, and b) improving the production objectives such as yield, rate, which reduces industries production costs.

Crystal growth performance objectives vary depending on the material type. Thus, one typically considers the requirements for compound materials separately from that of silicon. However, viewed from a systems point of view, while the specific details are different, one can exploit the similarities of the process physics so that advances in control architecture for one system are applicable to the other. In general, what makes it difficult to achieve the multiple objectives is that one must understand the coupling between the inputs, process physics, and outputs in order to explicitly take this coupling into account in the controller design. Thus for example, dislocations are created both at the growth interface as well as throughout the boule. The objective of the control related modeling work, therefore, is to develop a more explicit formulation of the coupling so it can be explicitly included in the control design.

In contrast, the current control structure utilizes real-time feedback control of pull rate, Vp, and heater power, Pin, to maintain diameter control, while other objectives are achieved by "open-loop" experimentally determined trajectories for crystal and crucible rotation rate and design of the hot zone. As such, there is no explicit consideration and control coordination of the process-material objectives. The conventional diameter control system is a cascaded controller, whereby the pull rate is adjusted to maintain the desired diameter, and the pull rate is compared to a desired pull rate trajectory to generate an error signal which is used to adjust the heater power. This is a classic feedback system, acting after the error has occurred.

**Experimental benchmarks and modeling.** We have developed and analyzed a realistic equipment model of a commercial scale puller, analyzed data sets for actual growth runs in commercial scale equipment to both verify our model and gain direct insight into control issues, and utilized the combined equipment-process model to evaluate a new control architecture. This analysis suggests that a more direct control strategy of maintaining the melt temperature would a) more directly prevent adverse growth conditions, and b) enable one to operate "closer to the edge" (i.e. limit the pull rate reduction) and achieve an increase in process productivity. This result has led us to a new control structures that achieves better performance over the conventional cascaded control.

## 3. PERSONNEL SUPPORTED

**Principal Investigators:**

Dr. V. Prasad, Director of the Consortium, Professor of Mechanical Engineering and Materials Science and Eng., Associate dean of College of Engineering and Applied Sciences. SUNY at Stony Brook.

Dr. M. Dudley, Co-PI, Professor and Chairman, Dept. of Materials Science and Engineering, USB.

Dr. J.E. Flaherty, Co-PI, Amos Eaton Professor of Computer Science, RPI.

Dr. M. Gevelber, Co-PI, Associate Professor of Manufacturing Engineering, Boston University.

Dr. J. Glimm, Co-PI, Distinguished Professor and Chairman, Dept. of Applied Mathematics and Statistics, USB.

Dr. M. Gunzburger, Co-PI, Professor and Chairman, Dept. of Mathematics, Iowa State Univ.

Dr. F. Ladeinde, Co-PI, Associate Professor of Mechanical Engineering, USB.

Dr. A. Maniatty, Co-PI, Clare Boothe Luce Assistant Professor of Mechanical Engineering, RPI.

Dr. M.H.N. Naraghi, Co-PI, Professor of Mechanical Engineering, Manhattan College.

Dr. M.S. Shephard, Co-PI, S.A. and E.C. Johnson Professor of Engineering and Director, Scientific Computing Research Center, RPI.

Dr. J. Turner, Co-PI, Associate Professor of Mathematics, Arizona State University.

**Other Associated Faculty:**

Dr. S. Adjerid, Research Associate Professor, Computer Science (RPI) and now Associate Professor (VPISU)

Dr. D.J. Larson, Research Professor, Materials Science and Engineering (USB)

Dr. F. Tangerman, Visiting Asst. Professor, Applied Mathematics (USB)

Dr. H. Zhang, Asst. Professor, Mechanical Engineering (USB)

Dr. L. Zheng, Asst. Professor, Mechanical Engineering (USB)

Dr. A. Varshney, Professor, Computer Science (USB)

Dr. Kenneth Jensen, Assistant Professor (RPI)

Dr. D. A. Drew, Eliza Ricketts Foundation Professor of Mathematics (RPI)

Dr. Dan Givoli, Associate Professor, Aeronautical Engineering (Technion)

Dr. Janet Peterson, Professor, Dept. of Mathematics, Iowa State Univ.

**Research Scientists/Post Doctoral Fellows:**

Dr. A. Chatterjee, Research Associate, Mechanical Engineering (USB)
Dr. Q. S. Chen, Research Scientist, Mechanical Engineering (USB)
Dr. W. Chui, Post-doctoral Fellow, Applied Mathematics (USB)
Dr. G. Dhanaraj, Research Scientist, Materials Science (USB)
Dr. D. Mishra, Research Scientist, Mechanical Engineering (USB)
Dr. A. Roy, Research Scientist, Mechanical Engineering (USB)
Dr. A.K. Saha, Post-doctoral Fellow, Mechanical Engineering (USB)
Dr. G.-X. Wang, Research Scientist, Mechanical Engineering (USB)
Dr. J.-Y. Zhao, Post-doctoral Fellow, Materials Science & Engineering (USB)
Dr. John Burkardt, Post-doctoral Fellow, Mathematics (ASU/ISU)
Dr. Erzin Ozugurlu, Post-doctoral Fellow, Mathematics (ASU/ISU)
Dr. Ajit Shenoy, Post-doctoral Fellow, Mathematics (ASU/ISU)
Dr. Lazarus Tenek, Post-doctoral Fellow, Mathematics (ASU/ISU)
Dr. Yih-Farn Chen, Post-doctoral Fellow (BU)
Mr. Mark Beall, Research Engineer (RPI)
Dr. Ottmar Klaas, Research Associate (RPI)
Dr. Yong Liu, Postdoctoral Fellow (RPI)
Dr. Kang Wang, Postdoctoral Fellow (RPI)

**Graduate Students:**

A. Chatterjee, Mechanical Engineering (USB)
H. Chung, Materials Science and Engineering (USB)
M. Ferland, Mechanical Engineering (USB)
W. Garber, Applied Mathematics (USB) (AASERT)
V. Gupta, Computer Science (USB)
I. Jafri, Mechanical Engineering (USB)
P. Lutjen, Mechanical Engineering (USB) (AASERT)
R. Ma, Mechanical Engineering (USB)
D. Mukherjee, Mechanical Engineering (USB)
A. Pal, Mechanical Engineering (USB)
S. Pendurti, Mechanical Engineering (USB)
A. Purwar, Mechanical Engineering (USB)
R. Sahoo, Mechanical Engineering (USB)
D. Sun, Mechanical Engineering (USB)
T. Zhang, Mechanical Engineering (USB)
J. Xu, Mechanical Engineering (USB)
R. Garimella, Computer Science (RPI)
R. Kalan, Mechanical Engineering (RPI)

H. Li, Mechanical Engineering (RPI)

J. Teresco, Computer Science (RPI) (AASERT) (Assistant Professor, Williams College)

W. Turner, Ph.D., Computer Science (RPI) (Currently Staff Scientist, GE, CR&D)

D. Wang, M.S., Computer Science (RPI)

L. Ziantz, Ph.D. (RPI) (Currently Assistant Professor, Dickenson College)

A.E. Livingston, Mathematics Department, (ASU)

A. Neghabat, Mechanical Engineering (Manhattan College)

E. M. Nunes, Mechanical Engineering (Manhattan College)

V. Rabinovich, Manufacturing Engineering (BU)

Z. Ren, Manufacturing Engineering (BU)

D. Wilson, Manufacturing Engineering (BU)

**Undergraduate Students:**

W. Clark, Mechanical Engineering (USB)

E. Hini, Science Major (USB)

P. Mohanty, Mechanical Engineering (USB)

N. Mouzakitis, Mechanical Engineering (USB)

N. Nemick, Mechanical Engineering (USB)

C. Truong, Materials Science and Engineering (USB)

M. Whiten, Mechanical Engineering (USB)

S. Barsi, Mechanical Engineering (Manhattan College)

K. Kean, Mechanical Engineering (Manhattan College)

A.J. Masteropietro, Mechanical Engineering (Manhattan College)

**Collaborators:**

Dr. D.F. Bliss, USAF Reseach Laboratory, Hanscom

Dr. G. Muller, University of Erlangen-Nurenberg, Germany

Dr. S. Balint, University of the West Timisoara, Romania

**Consultant:**

Dr. D.T.J. Hurle, Visiting Professor, School of Physics and Mathematics (Bristol, UK)

## 4. PUBLICATIONS

**Book Chapter**

1. Dhanaraj, G., Huang, X.R., Dudley, M., Prasad, V., and Ma, R.-H., Silicon Carbide Crystals - Part I: Growth and Characterization, in *Crystal Growth for Modern Technology*, K. Byrappa and T. Ohachi, eds., Noyes Publications, NJ, (2001).
2. Q. S. Chen, V. Prasad, H. Zhang, M. Dudely, and R.-M. Ma, Silicon Carbide Crystals - Part II: Process Physics and Modeling, in *Crystal Growth for Modern Technology*, edited by K.Byrappa and T.Ohachi, Noyes Publications, NJ, 2001.
3. H. Zhang and V. Prasad, "Modeling of High Pressure Liquid-Encapsulated Czochralski Processes," *in **Modeling of Transport Phenomena in Crystal Growth*** (Eds: J. S. Szmyd and K. Suzuki), pp. 323-362, WIT Press, Southampton, UK, 2000.

4. G.-X. Wang, and V. Prasad, "Rapid Solidification: Fundamentals and Modeling," ***Annual Review of Heat Transfer,*** ed. C.-L. Tien, Begell House Publishing, New York, Vol. XI, pp. 207-305, 2000.
5. V. Prasad, H. Zhang and A. Anselmo, "Transport Phenomena in Czochralski Crystal Growth Processes," ***Advances in Heat Transfer***, Vol. 30, pp. 313-435, Academic Press, 1997.
6. V. Prasad and H. Zhang, "Challenging Issues in Bulk Crystal Growth Modeling," ***Ceramic Transactions***, Vol. 60, pp. 3-36, The American Ceramic Society, Westerville, OH, 1996.

**Journal Publications:**

1. E.M. Nunes, V. Modi, and M.H.N. Naraghi, "Radiative Transfer in Arbitrarily Shaped Axisymmetric Enclosures with Anisotropically Scattering Media," ***International Heat and Mass Transfer Journal*** Vol. 43, pp. 3275-3285, 2000.
2. E.M. Nunes, M.H.N. Naraghi, H. Zhang and V. Prasad, "A Volume Radiation Heat Transfer Model for Czcralski Crystal Growth Processes," ***Journal of Crystal Growth*** (submitted).
3. E.M. Nunes, and M.H.N. Naraghi, "Numerical Model for Radiative Heat Transfer Analysis in Arbitrarily Shaped Axisymmetric Enclosures," ***Numerical Heat Transfer***, Part A, Vol. 33, pp. 495-513, 1998.
4. R. Kalan, and A. M. Maniatty, "Micromechanical based constitutive relations for modeling the bulk growth of single crystal InP," ***J. Crystal Growth*** (accepted).
7. D. Bliss, G. Bryant, R. Lancto, J. Zhao, M. Dudley, V. Prasad, and H. Zhang, "Assessment of the Necking Process as a Strategy for Dislocation Density Reduction in MLEC Crystal Growth of Sulfur-Doped InP," ***J. Crystal Growth*** (submitted).
8. Q.-S. Chen, H. Zhang, V. Prasad, C.M. Balkas and N.K. Yushin, Modeling of heat transfer and kinetics of physical vapor transport growth of silicon carbide crystals, ***J. of Heat Transfer*** (in press).
9. Y. P. Wan, H. Zhang, X.-Y. Jiang, S. Sampath and V. Prasad, "Role of solidification, substrate temperature and Reynolds number on droplet spreading in thermal spray deposition: measurements and modeling," ***Journal of Heat Transfer***, Vol. 123, pp. 382-389, 2001.
10. Q.-S. Chen, H. Zhang and V. Prasad , Heat Transfer and Kinetics of Bulk Growth of Silicon Carbide, ***J. of Crystal Growth***, Vol. 230/1-2, pp 239-246, 2001.
11. V. Prasad, Q.-S. Chen and H. Zhang, A Process Model for Silicon Carbide Growth by Physical Vapor Transport, ***J. of Crystal Growth***, Vol. 229/1-4, pp. 510-515, 2001.
12. Q.-S. Chen, R.-H. Ma, H. Zhang, V. Prasad, C.M. Balkas and N.K. Yushin, Modeling of transport processes and kinetics of silicon carbide bulk growth, ***J. of Crystal Growth***, Vol. 225/2-4, pp 299-306, 2001.
13. Q.-S. Chen, H. Zhang, V. Prasad, C.M. Balkas, N.K. Yushin and S. Wang, Kinetics and modeling of sublimation growth of silicon carbide bulk crystal, ***J. Crystal Growth***, Vol. 224/1-2, pp. 101-110, 2001.
14. R.-H. Ma, Q.-S. Chen, H. Zhang, V. Prasad, C.M. Balkas and N.K. Yushin, Modeling of silicon carbide crystal growth by physical vapor transport method, ***J. Crystal Growth***, Vol. 211 (1-4), pp. 352-359, 2000.
15. A. Roy, B. Mackintosh, J.P. Kalejs, Q.-S. Chen, H. Zhang and V. Prasad, A numerical model for inductively heated cylindrical tube growth system, ***J. Crystal Growth***, Vol. 211, pp. 365-371, 2000.

16. T. Zhang, F. Ladeinde, and V. Prasad, "Turbulent Convection in Large Czochralski Melt," ***Journal of Heat Transfer,*** Vol. 121, pp. 1027-1041, 1999.

17. Y. F. Zou, G. X. Wang, H. Zhang, and V. Prasad, "Mechanisms of Thermal-Solutal Transport and Segregation in a High Pressure Liquid-Encapsulated Czochralski System," ***Journal of Heat Transfer***, Vol. 121, pp.148-159, 1999.

18. Q.-S. Chen, W.-R. Hu, and V. Prasad, Effect of liquid bridge volume on the instability in small-Prandtl-number half zones, ***J. Crystal Growth***, Vol. 203, pp. 261-268, 1999.

19. Q.S. Chen, V. Prasad, A. Chatterjee and J. Larkin, A porous media-based transport model for hydrothermal growth, ***J. Crystal Growth***, Vol. 198/199, pp. 710-715, 1999.

20. Q.-S. Chen, V. Prasad and A. Chatterjee, Modeling of fluid flow and heat transfer in a hydrothermal crystal growth system: use of fluid-superposed porous layer theory, ***J. Heat Transfer***, 1999, Vol. 121, pp. 1049-1058.

21. H. Zhang, L.L. Zheng, V. Prasad, and D. J. Larson, Jr., 1998, "Diameter Controlled Czochralski Growth of Silicon Crystal," ***Journal of Heat Transfer***, Vol. 120, pp. 874-882.

22. H. Zhang, L.L. Zheng, V. Prasad, and D. J. Larson, Jr., 1998, "Local and Global Simulations of Bridgman and Czochralski Crystal Growth," ***Journal of Heat Transfer***, Vol. 120, pp. 865-873.

23. H. Zhang, L.L. Zheng, V. Prasad, and T.Y. Hou, "A Curvilinear Level set Formulation for Highly Deformable Free Surface Problems with Application to Solidification" ***Numerical Heat Transfer***, Vol. B34, pp. 1-20, 1998.

24. T. Zhang, G.X. Wang, H. Zhang, F. Ladeinde and V. Prasad, "Turbulent Transport of Oxygen in the Czochralski Growth of Large Silicon Crystals," ***J. of Crystal Growth,*** Vol. 198/199, pp. 141-146, 1998.

25. H. Chung, M. Dudley, D. J. Larson, Jr., D. T. J. Hurle, D. F. Bliss and V. Prasad "The Mechanism of Growth-Twin Formation in Zincblende Crystals: New Insights from a Study of Magnetic Liquid Encapsulated Czochralski Grown InP Single Crystals", ***J. Crystal Growth***, 187, 9-17, (1998).

26. M. Dudley, B. Raghothamachar, Y. Guo, X.R. Huang, H. Chung, D. T. J. Hurle, and D. F. Bliss, "The Influence of Polarity on Twinning in Zincblende Structure Crystals: New Insights from a Study of Magnetic Liquid Encapsulated, Czochralski Grown InP Single Crystals" ***J. Crystal Growth***, 192, 1-10, (1998).

27. W. Chui, J. Glimm, F. Tangerman, H. Zhang, and V. Prasad, *A Parallel Algorithm for Multizone, Multiphase Systems with Application to Crystal Growth*, ***J. Crystal Growth***, Vol 180, No. 3-4, pp 534--542, 1997.

28. W. Garber, F. Tangerman. *Parallel Computation of Radiative Heat Transfer in an Axisymmetric Closed Chamber: An Application to Crystal Growth*, Submitted to ***J. Crystal Growth***, 2000.

29. M. Gevelber, "Process Control", in ***the Encyclopedia of Electrical and Electronic Engineering***, John Wiley & Sons, 1999.

30. S. Adjerid, B. Belguendouz, and J.E. Flaherty, "A Posteriori Finite Element Error Estimation for Diffusion Problems", ***SIAM J. Sci. Comput.***, (in press).

31. M.W. Beall and M.S. Shephard, "An object-oriented framework for reliable numerical simulations", ***Engineering with Computers***, 15, 61-72, 1999.

32. H.L. DeCougny and M.S. Shephard, "Parallel volume meshing using face removals and hierarchical repartitioning", ***Comp. Meth. Appl. Mech. Engng.***, 174 (1999), 275-298.

33. R. Wentorf, R. Collar, M.S. Shephard, and J. Fish, "Automatic modeling of complex woven mesostructures", ***Comp. Meth. Appl. Mech. Engng.***, 172 (1999), 273-291.

34. S. Adjerid, J.E. Flaherty, K. Jansen, and M.S. Shephard, "Parallel Finite Element Simulations of Czochralski Melt Flows", in S.N. Atluri and P.E. O'Donoghue, Eds., ***Modeling and Simulation Based Engineering***, 1, Tech Science Press, Palmdale, 821-826, 1998.

35. Adjerid, S., Aiffa, A., Flaherty, J.E., Hudson, J.B., and Shephard, M.S., 1997, 'Modeling and Adaptive Numerical Techniques for Oxidation of Ceramic Composites', ***Ceramic Engng. And Sci. Procs.***, Vol. 18, pp. 315-322.

36. M.S. Shephard, H.L. de Cougny, R.M. O'Bara, and M.W. Beall, "Automatic grid generation using spatially-based trees", in J.F. Thompson, B.K. Soni, and N.P. Weatherill, Eds., ***CRC Handbook of Grid Generation,*** CRC Press, Boca Raton, 15.1-15.21, 1999.

37. J. D. Teresco, M. W. Beall, J. E. Flaherty and M. S. Shephard. "A hierarchical partition model for adaptive finite element computations," ***Comp. Meth. Appl. Mech. Engrg.***, 184(2000), 269-285.

38. S. Adjerid, M. Aiffa, and J.E. Flaherty, "Hierarchical finite element bases for triangular and tetrahedral elements, ***Comp. Meths. Appl. Mech. Engrg.***, 2001, to appear.

39. W.D. Turner and J.E. Flaherty, "Toward the design of a parallel, linear algebraic system, ***J. Par. Distrib. Comput.***, submitted, 2000.

40. M.S. Shephard, "Meshing environment for geometry-based analysis", ***Int. J. Numer. Meths. Engng.,*** 47(1-3):169-190, 2000.

41. R. Garimella and M.S. Shephard, "Boundary layer mesh generation for viscous flow simulations in complex geometric domains", ***Int. J. Numer. Meths. Engng.,*** 49(1-2):193-218, 2000.

42. R. Joslin, M. Gunzburger, G. Erlebacher, M. Hussaini, and R. Nicolaides, An automated methodology for optimal flow control with an application to transition delay; ***AIAA J.*** 35, 1997, 816-824.

43. J. Appel and M. Gunzburger, Difficulties in sensitivity alculations for flows with discontinuities, ***AIAA J.*** 35, 1997, 842-848.

44. Y. Cao, M. Gunzburger, and J. Turner, The exact controllability of systems governed by linear parabolic equations, ***J. Math. Anal. Appl.***, 215, 1997, 174-189.

45. Fursikov, M. Gunzburger, and L. Hou, Boundary value problems and optimal boundary control for the Navier-Stokes system: the two-dimensional case, ***SIAM J. Cont. Optim.*** 36, 1998, 852-894.

46. L. Hou, S. Manservisi, M. Gunzburger, and Y. Yan; Computations of optimal controls for incompressible flows, **Int. J. Comp. Fluid Dyn.** 11, 1998, 181-191.

47. M. Gunzburger, H.-K. Lee, and J. Peterson; An optimization based domain decomposition method for partial differential equations, ***Comp. Math. Appl.*** 37, 1999, 77-93.

48. M. Gunzburger; Sensitivites, adjoints, and flow optimization, ***Inter. J. Num. Meth. Fluids.*** 31, 1999, 53-78.

49. M. Gunzburger and S. Manservisi; The velocity tracking problem for Navier-Stokes flows with bounded distributed control, ***SIAM J. Cont. Optim.*** 37, 1999, 1913-1945.

50. M. Gunzburger, M. Heinkenschloss, and H.-K. Lee; Solution of elliptic partial differential equations by an optimization-based domain decomposition method, ***Appl. Math. Comp.*** 113, 2000, 111-139.

51. M. Gunzburger and S. Manservisi; Analysis and approximation of the velocity tracking problem for Navier-Stokes flows with distributed control, ***SIAM J. Numer. Anal.*** 37, 2000, 1481-1512.

52. M. Gunzburger and H.-K. Lee; An optimization-based domain decomposition method for the Navier-Stokes equations, ***SIAM J. Numer. Anal.*** 37, 2000, 1455-1480.

53. M. Gunzburger and S. Manservisi; Analysis and approximation for linear feedback control for tracking the velocity in Navier-Stokes flows, ***Comp. Meth. Appl. Mech. Engrg.*** 189, 2000, 803-823

54. Q. Du and M. Gunzburger; A gradient method approach to optimization-based multidisciplinary simulations and nonoverlapping domain decomposition algorithms, ***SIAM J. Numer. Anal.*** 37, 2000, 1513-1541.

55. M. Gunzburger and S. Manservisi; The velocity tracking problem for Navier-Stokes flows with boundary control, ***SIAM J. Cont. Optim.*** 39, 2000, 594-634.

56. M. Gunzburger and S. Manservisi; A variational inequality formulation of an inverse elasticity problem, ***Appl. Numer. Math.*** 34, 2000, 99-126.

57. M. Gunzburger and O. Emanouilov; Optimal control of stationary, low Mach number, highly nonisothermal viscous flows, ***ESAIM:COCV*** 5, 2000, 477-500.

58. On a shape control problem for the stationary Navier-Stokes equations, ***Math. Model. Numer. Anal.*** 34, 2000, 1233-1258.

59. M. Gunzburger; Adjoint equation-based methods for control problems in viscous, incompressible flows; to appear in ***Flow, Turbul., Comb.***

60. M. Gunzburger, E. Ozugurlu, J. Turner, and H. Zhang; Controlling transport phenomena in the Czochralski crystal growth process, submitted.

61. J. Burkardt, M. Gunzburger, and J. Peterson ; Insensitive functionals, inconsistent gradients, spurious minima, and regularized functionals in flow optimization problems, submitted.

**Conference Proceedings and Presentations:**

1. Q.-S. Chen, H. Zhang, and V. Prasad, Role of Thermocapillary Force in Silicon Czochralski Growth, ***The Thirteenth American Conference on Crystal Growth & Epitaxy (AACGE-13)***, August 12-16, 2001, Burlington, Vermont.

2. Q.-S. Chen, V. Prasad, H. Zhang, C.M. Balkas and N.K. Yushin, Physical phenomena and growth behavior of silicon carbide crystals, ***The Thirteenth International Conference on Crystal Growth in Conjunction with the Eleventh International Conference on Vapor Growth and Epitaxy (ICCG-13/ICVGE-11)***, 30 July - 4 August 2001, Kyoto, Japan.

3. V. Prasad, Q.-S. Chen and H. Zhang, A Process Model for Silicon Carbide Growth by Physical Vapor Transport, ***The 1st Asian Conference on Crystal Growth and Crystal Technology (CGCT-1 )***, August 29 - September 1, 2000, Sendai, Japan.

4. Q.-S. Chen, H. Zhang and V. Prasad , Heat Transfer and Kinetics of Bulk Growth of Silicon Carbide, ***3rd International Workshop on Modeling in Crystal Growth***, September 27-29, 2000, Stony Brook, New York, USA.

5. Q.-S. Chen, R.-H. Ma, H. Zhang, V. Prasad, C.M. Balkas and N.K. Yushin, Modeling of transport processes and kinetics of silicon carbide bulk growth, ***12th American Conference on Crystal Growth & Epitaxy***, August 13-18, 2000, Vail, Colorado.

6. H. Zhang, L.L. Zheng and V. Prasad, "Numerical Simulation of Dynamical Czochralski Growth with Control", ***IUMRS-ICAM' 99***, China.

7. G.X. Wang and V. Prasad, "Microscale Heat and Mass Transfer and Non-equilibrium Phase Change in Rapid Solidification", ***IUMRS-ICAM' 99***, China.

8. Bliss, D., Bryant, G., Lancto, R., Zhao, J., Dudley, M., Prasad, V., and Zhang, H., "Dislocation Generation and Propagation Near the Seed-Crystal Interface During MLEC Crystal Growth OF Sulfur -Doped InP", ***Proceedings of Eleventh International Conference on InP and Related Materials***, Davos, Switzerland (1999).

9. A. Chatterjee, D. Sun, V. Prasad, "Three Dimensional Modeling of High Pressure Crystal Growth," ***American Conference for Crystal Growth***, Tucson, AZ, 1999.

10. Lutjen, P., Clark, W., and Prasad, V., "Liquid Crystal Thermography and Scanning Flow Tomoscopy for Three-Dimensional Temperature Field Measurement," ***National Heat Transfer Conference,*** Albuquerque, 1999.

11. S. Pendurti, H. Zhang, V. Prasad, "Modeling Dislocation Generation in the Czochralski System", ***American Conference for Crystal Growth***, Tucson, AZ, 1999.

12. R.-H. Ma, Q.-S. Chen, H. Zhang, V. Prasad, C.M. Balkas and N.K. Yushin, Modeling of silicon carbide crystal growth by physical vapor transport method, ***11th American Conference on Crystal Growth & Epitaxy***, August 1-6, 1999, Tucson, Arizona.

13. A. Roy, Q.-S. Chen, H. Zhang and V. Prasad, An integrated model for electromagnetic field and heat transfer in cylindrical silicon tube growth by EFG method, ***the 1999 International Mechanical Engineering Congress & Exposition***, DE-Vol. 104, Electronics Manufacturing Issues, pp. 9-14, Nashville, Tennessee, Nov. 14-19, 1999.

14. A. Roy, B. Mackintosh, J.P. Kalejs, Q.-S. Chen, H. Zhang and V. Prasad, A numerical model for inductively heated cylindrical tube growth system, ***11th American Conference on Crystal Growth & Epitaxy***, August 1-6, 1999, Tucson, Arizona.

15. Q.-S. Chen, H. Zhang, V. Prasad, C.M. Balkas and N.K. Yushin, A system model for silicon carbide crystal growth by physical vapor transport method, ***Proceedings of the 33rd National Heat Transfer Conference***, NHTC99-222, pp. 1-8, August 15-17, 1999, Albuquerque, NM.

16. Q.S. Chen, A. Pal, V. Prasad and D. Bliss, Growth kinetics and solute transfer in a hydrothermal crystal growth process, ***11th American Conference on Crystal Growth & Epitaxy***, August 1-6, 1999, Tucson, Arizona.

17. Zhang, T., Wang, G. X., Zhang, H., Ladeinde, F., and Prasad, V., 1998, "Oxygen Transport in Czochralski Growth of 300 mm Diameter Silicon Crystal," ***Proc. of Electrochem. Soc.: Symposium on High Purity Silicon V***, Boston, 1998.

18. Ladeinde, F., Prasad, V., and Larson, D.J., "On the Missing Link Between Melt Convection and Crystal Quality," ***12th International Conference on Crystal Growth***, Jerusalem, Israel, 1998.

19. Jafri, I., Prasad, V., Gupta, K., Bliss, D. F., and Chandra, M., "Design of a New High Pressure Crystal Growth System for III-V Compound Crystals," ***12th International Conference on Crystal Growth***, Jerusalem, Israel, 1998.

20. Zhang, H., Wang, G. X., Bliss, D. F., Bryant, G., Iseler, G. W., and Prasad, V., "Global Simulation and Temperature Measurements of InP Growth," ***12th International Conference on Crystal Growth***, Jerusalem, Israel, 1998.

21. Chatterjee, A. and Prasad, V., "Three-dimensional Simulation of Czochralski Crystal Growth," ***12th International Conference on Crystal Growth***, Jerusalem, Israel, 1998.

22. Pendurti, S., Wang, G. X., and Prasad, V., "Effect of Thermal Boundary Conditions and the thickness of Encapsulation on Thermal Stress in As-Grown InP Crystal," ***12th International Conference on Crystal Growth***, Jerusalem, Israel, 1998.

23. Dudley, M., Chung, H., Larson, D.J., Jr., Hurle, D., Bliss, D.F., Prasad. V., Maniatty, A., and Kalan, R., "Post-Growth Studies of Interface Shape, Plastic Deformation and Growth Twin Formation in MLEC Grown, Sulfur-doped, <100> InP Single Crystals," ***12th International Conference on Crystal Growth***, Jerusalem, Israel, 1998.

24. Zhang, T., Wang, G.-X., Zhang, H., Ladeinde, F., and Prasad, V., 1998, "Oxygen Transport in Czochralski Growth of 300 mm Diameter Silicon Crystal," ***Proceeding of Electrochemical Society Symposium on High Purity Silicon V,*** Boston, 1998.

25. Bliss, D., Bryant, G., Jafri, I., Prasad, V., Gupta, K., Farmer, R., and Chandra, M., "A New High-Pressure System for Synthesis and Crystal Growth of Large Diameter InP," ***Ninth International Conference on Indium Phosphide and Related Materials***, Tsukuba, Japan, 1998.

26. Dudley, M., Raghothamachar, B., Guo, Y., Huang, X.R., Chung, H., Larson, D.J., Jr., Hurle, D.T.J., Bliss, D.F., Prasad, V., and Huang, Z., "The Mechanism of Twinning in Zincblende Structure Crystals: New Insights on Polarity Effects from a Study of Magnetic Liquid Encapsulated Czochralski Grown InP Single Crystals," *in* Applications of Synchrotron Radiation Techniques to Materials Science IV, S.M. Mini, D.L. Perry, S.R. Stock, and L.J. Terminello (Eds.), ***Materials Research Society Symposium Proceedings, Vol***. 524, 65-70, 1998.

27. Q.S. Chen, V. Prasad, A. Chatterjee, and J. Larkin, Modeling of solute transfer in a hydrothermal crystal growth process, ***The Eastern Regional Conference on Crystal Growth and Epitaxy***, Sept. 27-30, 1998, Atlantic city, NJ.

28. Q.S. Chen, V. Prasad, A. Chatterjee and J. Larkin, A porous media-based transport model for hydrothermal growth, ***12th International Conference on Crystal Growth***, July 26-31, 1998, Jerusalem, Israel.

29. Q.-S. Chen, V. Prasad and A. Chatterjee, Modeling of fluid flow and heat transfer in a hydrothermal crystal growth system: use of fluid-superposed porous layer theory, ***the 1998 International Mechanical Engineering Congress & Exposition***, Nov. 15-20, 1998, Anaheim, USA, HTD-Vol. 361-4, Proceeding of the ASME Heat Transfer Division, pp. 119-129.

30. Kalan, R. and Maniatty, A.M., "Indium Phosphide Constitutive Model Used in Crystal Growth," R. C. Picu and E. Krempl (eds.), ***Fourth International Conference on Constitutive Laws for Engineering Materials***, pp. 90-93, Rensselaer Polytechnic Institute, Troy, NY (1999).

31. A.M. Maniatty, "Stresses in Textured Thin Polycrystalline Films on Substrates," R. C. Picu and E. Krempl (eds.), ***Fourth International Conference on Constitutive Laws for Engineering Materials***, pp. 229-232, Rensselaer Polytechnic Institute, Troy, NY, 1999.

32. A.M. Maniatty, "Computational Modeling of Crystalline Materials," ***Yale University***, October 1998.

33. R. Kalan and A Maniatty, "Computational Model for Predicting Thermal Stresses During Crystal Growth," ***American Conference for Crystal Growth***, Tucson, AZ, 1999.

34. W. Garber and F. Tangerman, *Calculating Radiative Heat Transfer in an Axisymmetric Closed Chamber: An Application to Crystal Growth*, ***High Perfomance Computing, HPCU'99***, August 1999, Stony Brook, New York.

35. R. K. Sahoo, W. K. Chui, V. Prasad, F. Tangerman, and J. Glimm, *A Multizone Adaptive Parallel Algorithm for Melting and Solidification*, ***The 11th International Heat Transfer Conference***, Korea, June 1998.

36. W. Chui, J. Glimm, and F. Tangerman, *Parallel Simulations for Czochralski Crystal Growth*, Eastern Regional Conference on Crystal Growth, ***ACCGE/east-97***, Atlantic City, New Jersey, Sept 28 - Oct 1, 1997.

37. W. Chui, W. Garber, J. Glimm, and F. Tangerman, *Parallel Simulations for Crystal Growth*, ***Fourth U.S. National Congress on Computational Mechanics USNCCM IV***, San Francisco, California, August 4-9 1997.

38. W. Chui, J. Glimm, F. Tangerman, and H. Zhang, *Parallel Algorithm for Simulation of Crystal Growth Process*, ***SIAM Annual Meeting 1996***, Kansas City, Missouri, July 22-26, 1996.

39. W. Chui, J. Glimm, F. Tangerman, H. Zhang, and V. Prasad, *Parallel Computations for Crystal Growth Modeling*, ***The Tenth American Conference on Crystal Growth***, Vail, Colorado, August 4-9, 1996.

40. W. Chui, J. Glimm, F. Tangerman, H. Zhang, and V. Prasad, *A Parallel Algorithm for Multizone, Multiphase Systems with Application to Crystal Growth*, ***The 2nd International Workshop on Modelling in Crystal Growth***, Durbuy, Belgium, October 13-16, 1996.

41. W. Garber and F. Tangerman, *Calculating Radiative Heat Transfer in an Axisymmetric Closed Chamber: An Application to Crystal Growth*", ***High Perfomance Computing, HPCU'99***, August 1999, Stony Brook, New York.

42. Y. Chen, Z. Ren, M. Gevelber, H. Zhang and V. Prasad, "High-order Model Based Control Analysis of Czochralski Process", ***12th International Conference on Crystal Growth***, Jerusalam, Israel, 1998.

43. Y. Chen, J. Jiang and M. Gevelber, "Process Modeling Analysis for Enhanced Control of INP Synthesis", ***12th International Conference on Crystal Growth***, Jerusalam, Israel, 1998.

44. Nunes, E.M., Naraghi, M.H.N., and Modi, V., "Radiative Transfer in Axisymmetric Bodies with Non-homogenous Media," to be presented at ***the 35th National Heat Transfer Conference***, Anaheim, California, June 10-12, 2001 (***paper # NHTC01-12233***).

45. Nunes, E.M., Naraghi, M.H.N., Zhang, H. and Prasad, V., "Numerical Simulation of Transport Processes During Czochralski Growth of YAG and BSO," ***American Conference for Crystal Growth***, Tucson, AZ, 1999.

46. Nunes, E.M., Naraghi, M.H.N., Zhang, H. and Prasad, V., "An Exchange Factor Formulation for Spectral Internal Radiation Heat Transfer Analysis of Czochralski Crystal Growth Processes," ***12th International Conference on Crystal Growth***, Jerusalem, Israel, 1998.

47. Nunes, E.M., Naraghi, M.H.N., Zhang, H., and Prasad, V., "A Volume Radiation Heat Transfer Model for Czochralski Crystal Growth Process," ***AIAA/ASME Heat Transfer Conference***, Denver, 1998.

48. Nunes, E.M. and Naraghi, M.H.N., "A Study of the Effects of Various Radiation Heat Transfer Parameters on the Czochralski Crystal Growth Processes," ***ACCGE/east-98***.

49. A. Neghabat, and M.H.N. Naraghi, "Analysis of Radiative Heat Transfer in Three-Dimensional Non-homogenous, Non-gray, and Anisotropic Scattering Media," ***Heat Transfer 1998***, Proceedings of 11th IHTC, Vol. 7, August 23-28, 1998, Kyongju, Korea.

50. J.E. Flaherty, "Parallel Adaptive Computation using Discontinuous Galerkin Methods," Department of Mathematical Sciences, ***University of Nevada at Las Vegas***, February 8, 2001.

51. J.E. Flaherty, "Parallel Adaptive Computation Using Discontinuous Galerkin Methods," Department of Applied Mathematics, ***Brown University***, Providence, February 11, 2000.

52. J.E. Flaherty, "Parallel Adaptive Solution of Conservation Laws by a Discontinuous Galerkin Method," workshop on ***A Posteriori Error Estimation and Adaptive Approaches in the Finite Element Method***, Mathematical Sciences Research Institute, University of California Berkeley, Berkeley, 3-14 April, 2000.

53. J.E. Flaherty, "Software for Parallel Adaptive DG Computation," special session on Discontinuous Galerkin Methods, ***Conference on Finite Elements in Flow Problems 2000***, The University of Texas at Austin, Austin, April 30 - May 4, 2000.

54. J.E. Flaherty, "Architecture-Dependent Finite Element Computation Using the Rensselaer Partition Model" and "Adaptive Discontinuous Galerkin Method with an Orthonormal Basis," Mini-Symposium on Parallel Adaptive Computations, ***Conference on p and hp Finite Element Methods: Mathematics and Engineering Practice (p-FEM 2000),*** Washington University, St. Louis, May 31 - June 2, 2000.

55. J.E. Flaherty, "Software for Parallel Adaptive Computation" and "A Posteriori Error Estimation for the Discontinuous Galerkin Method," ***Sandia National Laboratory***, Albuquerque, June 21, 22, 2000.

56. J.E. Flaherty and J.D. Teresco, "Software for parallel adaptive computation," in M. Deville and R. Owens, Eds., ***Proc. 16th IMACS World Cong. on Sci. Comput., Appl. Maths. and Simul.***, Paper 174--6, IMACS, Lausanne, 2000.

57. J.E. Flaherty, "Parallel Adaptive Computation using Discontinuous Galerkin Methods," Mathematical and Computational Sciences Division, ***National Institute of Standards and Testing***, Gaithersburg, September 26, 2000.

58. Flaherty, J.E., "Parallel Adaptive Solution of Conservation Laws by a Discontinuous Galerkin Method", ***International Symposium on Discontinuous Galerkin Methods Theory, Computation and Applications,*** Newport, 24-26 May 1999.

59. Flaherty, J.E., "Simple A Posteriori Error Estimates for Transient Problems," Minisymposium on A Posteriori Error Estimation and Reliability of FE Computations, ***Conference on The Mathematics of Finite Elements and Applications (MAFELAP)***, Brunel University, Uxbridge, 22-25 June 1999.

60. Flaherty, J.E., "Adaptive Computational Techniques for Partial Differential Equations", ANODE '98, ***University of Auckland***, Auckland, December 14-16, 1998.

61. M.S. Shephard, "Automation of large-scale simulations with emphasis on geometry-based issues", ***Technische Universtat Munchen***, Fakultat fur Bauingenieur und Vermessungswesen, Munich, Germany, March 6, 2000.

62. M.S. Shephard, "Automation of large-scale simulations with emphasis on geometry-based issues", ***Universtat Stuttgart, Institut fuer Baustatik***, Stuttgart, Germany, March 7, 2000.

63. M.S. Shephard, "Mesh Adaption for Curved Domains", ***Workshop on Adaptive FEM in Computational Mechanics***, Institute for Structural and Numerical Mechanics, Universitat Hannover, Hannover, Germany, March 9, 2000.

64. M.S. Shephard, "Automation of large-scale simulations with emphasis on geometry-based issues", Dept. of Mech. Eng. Seminar, ***Carnegie Mellon University***. Pittsburgh, PA, April 28, 2000.

65. M.S. Shephard, "Trellis - A geometry based adaptive analysis framework for a multi-processor environment", ***p and hp Finite Element Methods: Mathematics and Engineering Practice***, Washington University, St. Louis, MO, May 31, 2000.

66. M.S. Shephard, "Algorithm to generate p-version meshes for curved domains", ***p and hp Finite Element Methods: Mathematics and Engineering Practice***, Washington University, St. Louis, MO, June 2, 2000.

67. M.S. Shephard, "RPM: A System for Parallel Adaptive Scientific Computation", ***SIAM Conference on Scientific Computing***, Washington, DC, Sept. 21, 2000.

68. M.S. Shephard, "Mesh Adaption for Curved Domains", ***SIAM Conference on Scientific Computing***, Washington, DC, Sept. 24, 2000.

69. Shephard, M.S., "Simulation-Based Engineering: Providing the Tools," ***IBM Seminar, Poughkeepsie***, July 15, 1998.

70. Shephard, M.S., "Overview of Simulation-Based Engineering Efforts at SCOREC", ***Alcoa Development Center***, Pittsburgh, Aug. 17, 1998.

71. Shephard, M.S., "Open Issues in the Automatic Generation of Meshes", ***Meshing Roundtable***, Detroit, Oct. 27, 1998.

72. Shephard, M.S., Beall, M.W., and O'Bara, R.M., "Revisiting the elimination of the adverse effects of small model features in automatically generated meshes", ***Proc. 7th International Meshing Roundtable '98***, Report SAND 98-2250, Sandia Nat. Labs., Albuquerque, 119-131, 1998.

73. J. Turner, "Application of Optimal Control", *University of Cape Town*, South Africa, 1999.

74. J. Turner, "Modeling the MCz Crystal Growth Process", ***Second Annual Conference Minorities and Applied Mathematicians – Connections to National Laboratories***, Berkeley, 1998.

75. Y. Cao, M. Gunzburger, and J. Turner, On exact controllability and convergence of optimal controls to exact controls of parabolic equations; Optimal Control: Theory, Algorithms, and Applications, Kluwer, 1998, 67-83.

76. Fursikov, M. Gunzburger, and L. Hou, Optimnal Dirichlet control and inhomogeneous boundary value problems for the unsteady Navier-Stokes equations; Control of Partial Differential Equations, ***ESAIM Proceedings 4***, SMAI, Paris, 1998, 97-116

77. M. Gunzburger; Adjoint methods, Design Optimal et MDO, *Centre de Recherche en Calcul Applique,* Montreal, 1-25, 1998.

78. M. Gunzburger, Sensitivities in computational methods for optimal flow control; Computational Methods for Optimal Design and Control, Birkhauser, Boston, 1998, 197-236.

79. Gunzburger, H. Kim, and S. Manservisi; Shape design of channel flows for steady, incompressible flows; to appear in ***Proc. 39th Conf. Decision and Control***, IEEE.

80. M. Gunzburger, Introduction into mathematical aspects of flow control and optimization; to appear in Inverse Design and Optimisation Methods, von Karman Institute for Fluid Dynamics, Rhode-Saint-Genese, Belgium, 1997.

81. J. Appel and M. Gunzburger, Approximate solutions via ensitivities; to appear in Inverse Design and Optimisation Methods, von Karman Institute for Fluid Dynamics, Rhode-Saint-Genese, Belgium, 1997.

82. M. Gunzburger, Lagrange multiplier techniques; to appear in nverse Design and Optimisation Methods, von Karman Institute for Fluid Dynamics, Rhode-Saint-Genese, Belgium, 1997.

83. J. Appel and M. Gunzburger, Sensitivity calculation in flows with discontinuitites; AIAA Paper 96-2471, ***Proc. 14th AIAA Applied Aerodynamics Conference***, AIAA, 1996.

# 5 COLLABORATIONS/TRANSITIONS

## 5.1 Collaboration with Industry and Research Laboratories

Advanced Technology Materials, Inc., CT

ASE Americas, Inc., MA

Brookhaven National Laboratory, Upton, NY

CREE Research Inc., Durham, NC

General Semiconductor, Westbury, NY

GT Equipment Technologies, Nashua, NH

Kayex, Rochester, NY

Lockheed Martin, Schenectady, NY

NASA Lewis Research Center, Cleveland, OH

Sandia National Laboratories, Albuquerque, NM

Simmetrix Inc., Detroit, MI

Sterling Semiconductor, Inc., VA

USAF Research Laboratories, Hanscom and Wright Paterson

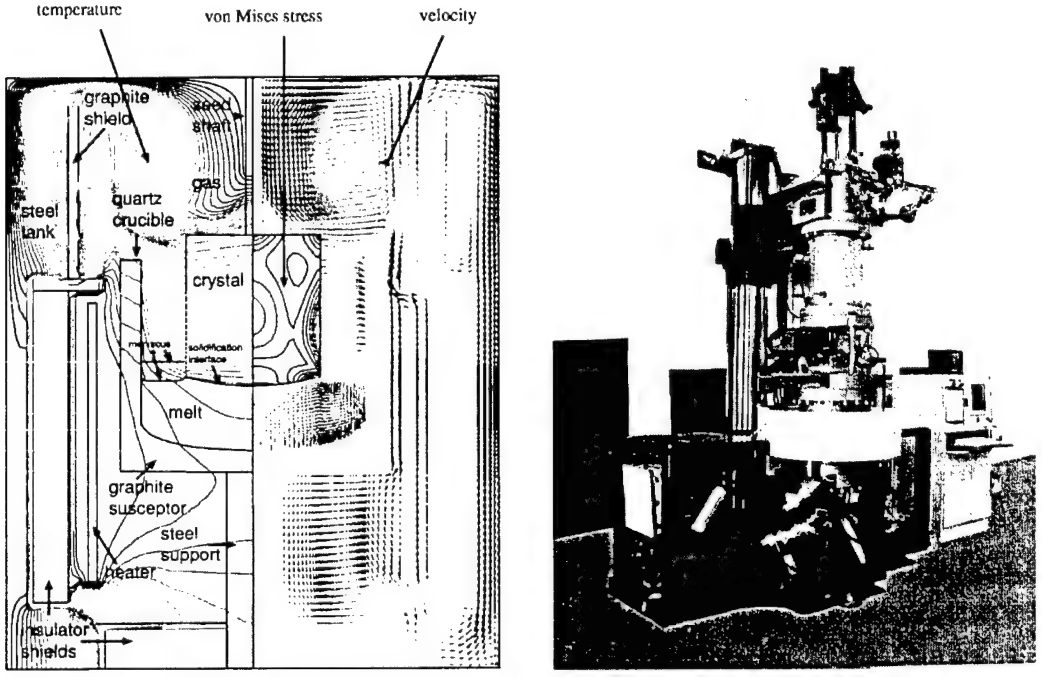
## 5.2 Transitions

As noted earlier, several new collaborative research programs in crystal growth and related areas (beyond that proposed originally) have been initiated by the Consortium researchers. It is important to state that these important initiatives would not have been possible without this MURI program. Following is a short description of the research goals and progress of selected industrial programs.

### 5.2.1 Design of Next Generation High Pressure Crystal Growth System

The Consortium has worked closely with GT Equipment Technologies (through an AFOSR STTR project) to design an advanced high pressure crystal growth system that is capable of producing large diameter, better quality InP crystals. The new furnace has a working pressure of up to 1200 psi (currently at 600 psi) and can accommodate a crucible of 6 inches in diameter with

a charge of 8 kg to enable the growth of up to 4 inches diameter InP crystals (present industry standard being 2 inches). At a later stage, the internal arrangement of the furnace can be easily modified to accommodate an eight-inch crucible to allow growth of 5-6" diameter crystals. To provide a better control of the synthesis and growth process, we have developed a novel design and have separated the growth chamber from the injector and seed chamber. This provides much better flexibility and operational ease. Global simulations have been very helpful in making design decisions. An InP growth system has been modeled by MASTRAPP (Fig. 1a). The new furnace design has much better thermal conditions (three heaters to provide better control of the melt), easy setup and convenient cleaning mechanism. Also, the phosphorous injector is heated separately to allow better control of the synthesis process. The proposed design has provisions for several sensors/actuators for sensing and feedback control of the synthesis and growth processes. The furnace has been fabricated and tested at the company's facility, and installed at USAF Research Laboratory at Hanscom. It can be used for growth experiments at much higher pressures. Another system has been set up at Stony Brook with the support from NSF (Fig. 1b). Several US companies have shown keen interests in the design of this furnace and they were consulted on a regular basis to develop a commercial system.




(a) (b)

**Figure 1.** (a) Simulated results for a high pressure liquid encapsulated Czochralski growth system and (b) newly designed high-pressure system for one-step in-situ synthesis and growth of III-V compounds installed at Stony Brook.

### 5.2.2 Modeling, Simulation and Design of Large Diameter Silicon Tube Growth

This project is presently underway at USB in collaboration with ASE Americas, Inc. Conventional melt growth technique such as float-zoning, Czochralski pulling, or Bridgman growth typically produce crystals in the form of cylindrical ingots. In many engineering applications, only a thin wafer of the crystal is required and hence, the ingot is cut into hundreds of slices. One of the undesirable consequences of this wafering is the surface damage which needs to be removed by appropriate etching and polishing. For large scale use, it is difficult to

produce thin wafers from an ingot without wasting 30 - 50 % of materials as kerf loss during the cutting process. Furthermore, the sawing process followed by polishing increases the costs of production. Such high costs of silicon wafers result in expensive solar cells, thereby grow polycrystalline silicon ribbons and tubes. For example, Ebara Corp. products 2 inches wide Si ribbon while ASE Americas grows octagonal silicon tubes. The octagon tube is cut in 4 X 4 inches wafers using laser.

Growth of large diameter silicon tube can bring further advancement of photovoltaic technology. The primary goal of the project is to work closely with ASE Americas, Inc. to develop a process for growing 50 cm diameter silicon tube of very small thickness (100 to 300 μm). The researchers of the AFOSR/DARPA Consortium of Crystal Growth Research is developing analytic and simulation tools to design and optimize the large diameter growth process as well as to assist them in thermal design of the growth system. A MASTRAPP based, comprehensive numerical model is has been developed which accounts for all modes of heat transfer, electromagnetic heating, capillary effects, solidification and interface dynamics, and thermoelastic stresses in as-grown tube. The model will serve several purposes, including a parametric study, basic understanding of the physical phenomena, design of experiments, process optimization and design of the new growth system. A scaling analysis has also been performed to evaluate the effects of various physical parameters. The Stony Brook researchers are actively participating in the discussions of the design of the new system and helping the ASE engineers in thermal analysis as needed. Using Stony Brook model, ASE has successfully designed and grown 50 cm diameter tube. This is a DOE project to bring innovations in photovoltaic technology and SUNY at Stony Brook is a partner with ASE Americas in this R & D endeavor. The success of this method will revolutionize the photovoltaic technology by producing much larger solar cells with enhanced cell efficiency than possible today with significant reduction in production cost.

### 5.2.3 Modeling of Silicon Carbide Crystal Growth by Physical Vapor Transport Method

A coupled heat and mass transfer model for bulk growth of silicon carbide crystals has been developed. The model incorporates conductive/radiative heat transfer, advective mass transfer and growth kinetics. This model has been developed in collaboration with two companies,

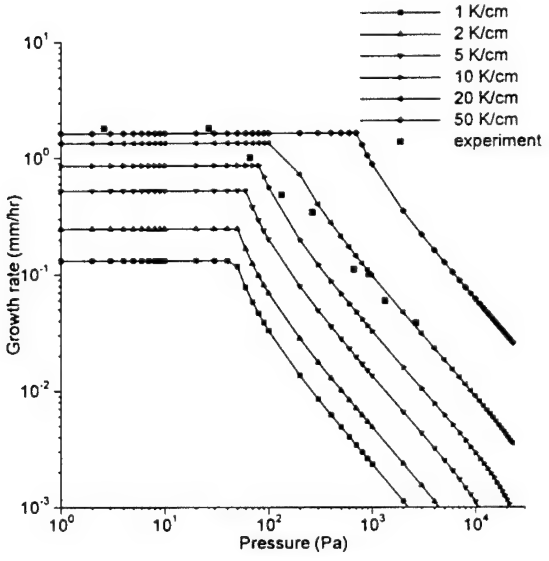



Figure 2a. Predicted growth rate with seed temperature of 2400 K. The experimental data are taken from [G. Augustine, et al. 1997] at seed temperature of 2398 K.

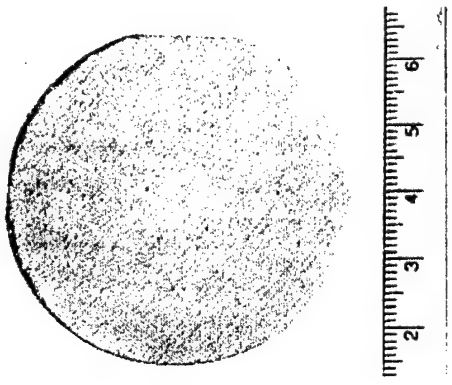


Figure 2b. 6H, 2" diameter wafer expanded from a Lely crystal by the modified Lely method in collaboration with Sterling semiconductor, Inc.

Sterling Semiconductor, Inc. and Advanced Technology Materials, Inc., to design upscaled systems for better control of thermal conditions that ultimately determine the growth conditions, its rate and crystal quality. Simulations have been performed based on the 1.5" and 2" diameter crystal designs provided by Sterling. The temperature distribution and growth rate are predicted and compared well with the measurements. The effects of pressure, temperature and temperature gradient on the growth rate have been studied. The model has helped in optimizing the thermal conditions in their 1.5" and 2" systems and enhancing the crystal quality. We also performed simulation based on the 1.5" system design provided by ATMI. The temperature distribution and the time transient effects for different ramp up schedules, etc. 45 minute and 90 minute, have been studied. Modeling and simulation has helped Sterling to grow 75 mm SiC crystals. Figure 2a presents predicted growth rate versus inert gas pressure for seed temperature of 2400 K. The experimental data were obtained by G. Augustine, et al. [1997] at seed temperature of 2398 K. Figure 2b shows a 2" diameter silicon carbide wafer grown from a Lely seed. Our model is the only simulation code available for dynamic modeling of SiC growth among the US institutions.

### 5.2.4 Modeling of Hydrothermal Crystal Growth

MASTRAPP3d is also being used to study the complex flow and heat and mass transfer and growth kinetics in hydrothermal crystal growth system. The thickness of vessel, the height of charge, the opening of baffle, the seed position and size, and the height of the heating portion of autoclave greatly influence the flow structure. The swirl flow, which consists of a strong flow in between the baffle and fluid/powder charge interface and a penetrating flow in the porous charge, plays an important role in transferring the saturated nutrient from the powder charge to the fluid part above the baffle. The nutrient is mainly transferred by the convective flow and the baffle opening directly regulates the mass transfer rate from the below-baffle fluid and porous charge part to the above-baffle fluid and seeds part. We have done several typical calculations of the flow and thermal fields on the hydrothermal crystal growth systems in the USAF RL at Hanscom and Sawyer Research Products (OH), which is the largest US producer of hydrothermally grown crystals. The former grows ZnO using hydrothermal method and the later grows quartz. The solute distributions in autoclaves have been given and growth rate decreases along the axis from the lower seed to the upper seed.

### 5.2.5 High Order Model and Control Analysis for Silicon Growth

High order model based numerical simulation (MASTRAPP) provides a numerical test bed to evaluate our control proposal in terms of revealing the detailed physics that the LOM does not provide, such as thermal stress and segregation. It also provides the basis for developing feedforward control trajectory. Our strategy here is to utilize feedback control to provide a local trim to the model based feedforward control.

In order to properly simulate control performance, MASTRAPP has been extended by adding several important features: (1) an efficient algorithm to find the equilibrium point; (2) a control subroutine to simulate cascaded PID control loop or other control algorithm; and (3) modifying the current version of MASTRAPP to account for realistic actuators/boundary conditions in a computationally tractable fashion to enable simulation of the entire batch dynamics. This latter effort includes adding: (1) a simplified radiative heat transfer model that accounts for batchwise disturbance; and (2) a representation of both conventional heater and advanced segmented heater options. The new model will be used to examine the traditional control performance and test our advanced control algorithm for improving crystal quality and controller performance, particularly in terms of interface shape.

We have also developed a systematic method to design the PID control gain that meets performance criteria such as zero steady state error, fast response, minimum over-shoot and minimum pulling rate variation. This method is based on a system identification algorithm that identifies the dominant eigenstructure from step response simulation using MASTRAPP. With

this practice, we will be able to examine the impact of the cascaded diameter control on other control objectives related to crystal quality, e.g., dislocation, twinning and segregation.

To test the model, a dynamic simulation of Si growth including melt convection has been performed (Fig. 3a) using constant values of the pull rate. Numerical studies show that a cylindrical shape of the crystal cannot be obtained without proper control. The predicted crystal/melt interface for an 8" diameter silicon at 24 cm growth length coincides with the interface revealed in the striation pattern of a MCLT map (Fig. 3b). The thermal stress distribution is determined by the interface shape and thermal gradient near the interface. This is the first time that a dynamic Cz growth with control has been presented that accounts for convection in the melt. Three control algorithms based on PID are developed and examined. Undamped oscillations of the shape of the crystal are obtained for the growth controlled by the radius. Damped oscillation is obtained for the growth controlled by the meniscus angle and by the combined radius and angle control. The dynamic response of the controlled Cz growth is examined by a diffusion model, a convection model, and a convection model with an axial magnetic field. The heat gains and losses are predicted at all interfaces. For the pull rate controlled growth, the conclusion obtained from the diffusion model can be extended to the convection model. The model has been extended to high-pressure growth of InP crystal.

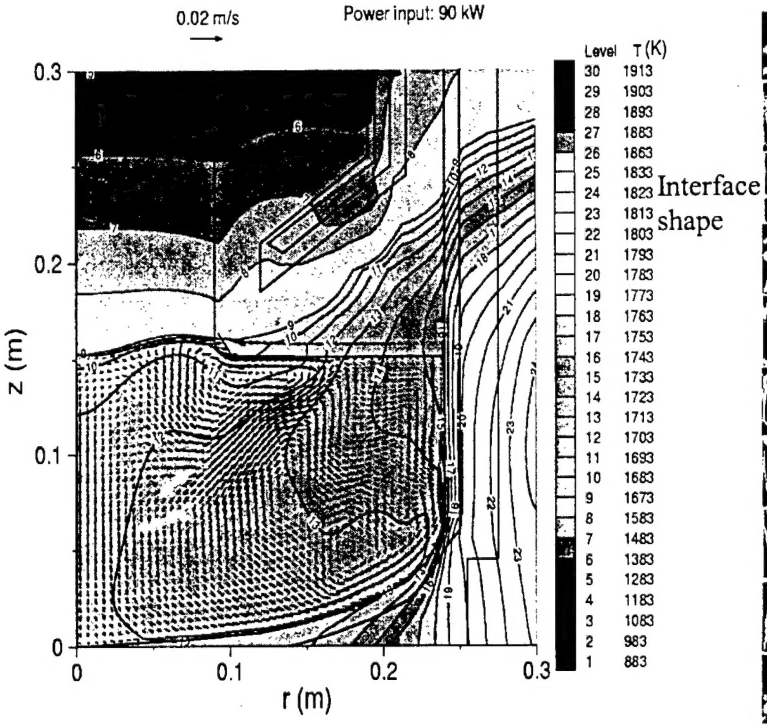



Figure 3a. Modeling of 8 inch Cz system. The rotation rates are 15 rpm for crystal, and 5 rpm for crucible, respectively. The crystal/melt interface is predicted which is comparable to the striation pattern of the MCLT map.

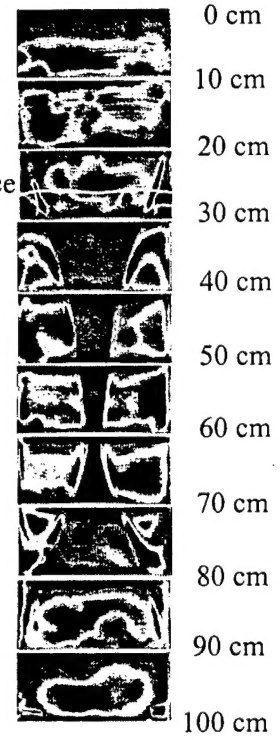



Figure 3b. MCLT map showing striation pattern produced by oscillatory melt flow.

### 5.2.6 An Integrated Approach to the Bulk III-Nitride Crystal Growth and Wafering

A MURI program involving investigators at NCSU, CU, Cornell, USB, ASU, NRL, and AFRL has been granted by ONR to study the bulk growth of aluminum nitride (AlN) and gallium nitride (GaN) single crystals. We will obtain all essential information on the growth systems and

processes used by NCSU, Cornell and CU. Based on this information, and we will develop an integrated model that will establish a cause-and-effect relationship between different parameters and observations concerned with the Nitrides growth. We will refine our continuum model using crystal evaluation data in terms of uniformity of growth, growth rate, morphology, stress management, and defect reduction. The results of these simulations will provide values for the temperature, temperature gradient, growth pressure and system geometry to NCSU, CU and Cornell, hereby giving them parameters for system optimization and allowing them to predict the nucleation and growth rate and shape of the growing crystal.

### 5.2.7 Simulation of Fiber Coating by CVD

Ceramic composites with alumina as fibers can be successfully used in high temperature applications, e.g., cylinder liners. Sapphire has been found to be an excellent fiber material for these applications. However, it suffers from severe problem of adhesion with the polymer that is used to produce composites. To overcome this difficulty, it is proposed to coat sapphire with β-alumina using chemical vapor deposition, which increases the adhesion at the interface. Flaherty and his co-workers have been working with the USAF Research Laboratory at Wright Paterson and Centric Engineering to simulate the CVD process for fiber coating using their FEM model.

### 5.2.8 Novel Methods for Polysilicon Production

Polysilicon forms the basic raw material that is used to grow single crystalline and polycrystalline Si for electronic, opto-electronic, photovoltaic, MEMS and many other devices. Currently, there is severe shortage of poly-Si and its price during 1993-1997 has increased by almost 100% and is expected to further increase if there is no major change in the fifty years old "Siemens process" that involves deposition of poly-Si on a slim Si-rod by CVD. There is only one US producer of poly-Si and the market is dominated by Asians and Europeans. The Consortium's industrial partner, GTi has proposed two patented (applied, Prasad as co-investigator) process technologies to substantially increase the production of poly-Si by retrofitting the existing equipment. Zhang and Prasad have worked with Gti on an NSF SBIR project to help simulate and design the new process using the MASTRAPP-based CVD model that has been developed recently to simulate epi-layer growth for General Semiconductor's high power device manufacturing processes.

### 5.2.9 Deposition by Thermal Spray

In thermal spray deposition, the solid particles when passed through plasma or other high temperature environments melt and the molten droplets then deposit on a cold substrate. Modeling and simulation of thermal spray deposition processes is very challenging because of the impact, spreading and non-equilibrium solidification of these molten splats, initially on the substrate and then on top of the previously deposited splats. Prasad, Zhang and Wang are working with the NSF Materials Center (MRSEC) on Thermal Spray at Stony Brook (H. Herman, Director with Prasad as a Co-PI) to develop an integrated process model. They have coupled MASTRAPP with Level Set Formulation and develop a novel numerical scheme for the processes involving highly deforming interfaces and multiple free surfaces together with phase-change. The thermal spray deposition model has already gone far beyond what was accomplished by the previous models. The LAVA (plasma code developed by INEEL) code has been further extended to model the particle-flame interaction.

### 5.2.10 Wiresaw Technology for Wafer Production

Wire sawing is an emerging technology for slicing large diameter thin wafers with minimal kerf (material) loss. In contrast to the current inner diameter (ID) saw (one wafer at a time), a wiresaw can slice several hundreds of wafers simultaneously. It is the only technology that can produce 300 *mm* (12") Si wafers that are required for next generation electronic device technology. Wiresaws can also be used to produce thin wafers (200–400 μm) of polycrystalline materials,

compound semiconductors, alumina, glass and other materials. The Consortium's focus on crystal growth and related processes has led to two research programs in the area of wiresaw technology at Stony Brook, (1) NSF university/industry program on fundamental aspects of the process including modeling, design and control, and (2) a DOE SBIR grant to GTi with USB as partner on industrial aspects of this technology including slurry management and environment impact. Our research on wire saw modeling and slurry recovery and reutilization has attracted international interest, and has also generated a patent (Prasad as co-inventor) for slurry recovery and reutilization.

## 6. NEW DISCOVERIES/INVENTIONS/PATENT DISCLOSURES

- MASTRAPP is considered to be the most advanced model in the world for simulation and virtual design of materials processes that involve phase-change, free surface movements, electromagnetic and thermoelectric fields. No other model can account for as many physical phenomena as incorporated into MASTRAPP.
- Interface shape, striation, defect generation and propagation have been related to flow field and thermal conditions in crystal growth.
- A comprehensive understanding of necking process for the reduction of defect density in InP crystals has been established with the help of experiments and efforts are underway to numerically model the same.
- A novel technology has been proposed for an energy efficient process to substantially increase polysilicon production.
- With USB's help Sterling Semiconductor was able to grow 75 mm SiC crystal.
- First ever growth of 50 cm diameter silicon tube of 200 μm thickness was reported by ASE in collaboration with USB.
- First transport model for hydrothermal growth.

## 7. HONORS/AWARDS

- E.M. Nunes received a three year NSF fellowship to pursue his doctorate degree.
- Antoinette M. Maniatty has been selected to be a member of the Defense Science Study Group for the years 2000, 2001.
- James Turner received the best paper award at the Fourth Biannual World Automation Congress held in Maui, Hawaii in June 2000 for the paper "An application of optimal control theory to crystal growth."
- M.S. Shephard was elected President of the U. S. Association of Computational Mechanics, 1999.
- J.E. Flaherty was elected a Fellow of the U.S. Association of Computational Mechanics, 1999.
- J.E. Flaherty was elected Secretary of the U. S. Association of Computational Mechanics, 1999.
- M.S. Shephard was elected a Fellow of the International Association of Computational Mechanics, 1998.
- Best paper awards to two students at AACG/East conference 1998.
- NSF CAREER award to Dr. H. Zhang to pursue research in modeling and prototyping of SiC growth and hydrothermal synthesis.
- Three Co-PIs, Drs. Maniatty, Gevelber, Ladeinde, were tenured and promoted.

- Two post-doctoral fellows, Dr. H. Zhang and Dr. G.-X. Wang were appointed tenure-track faculty at SUNY Stony Brook and University of Akron, respectively.
- An NSF research instrumentation (MRI) grant to establish *Integrated Crystal Growth and Wafer Manufacturing Research* Facility at Stony Brook, that will be unique in the world.
- An integrated approach to the bulk III-nitride crystal growth and wafering (ONR MURI project lead by North Carolina State University).
- Max Gunzburger has been appointed Distinguished Professor at Iowa State University, the highest honor given by the University.
- Prasad was appointed as leading professor at SUNY Stony Brook.
- Numerous invited presentations on crystal growth modeling at national and international meetings by Prasad.